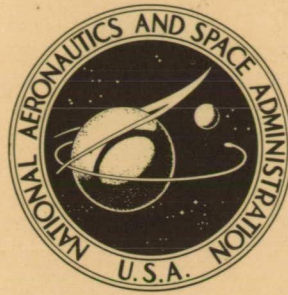


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# MICROWAVE SPECTRA OF SOME SULFUR AND NITROGEN COMPOUNDS

*by William F. White*  
*Langley Research Center*  
*Hampton, Va. 23665*



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# MICROWAVE SPECTRA OF SOME SULFUR AND NITROGEN COMPOUNDS

By William F. White  
Langley Research Center

## SUMMARY

The Langley Research Center has been engaged in the measurement and tabulation of microwave absorption spectra suitable for chemical analysis. Most of the measurements have been made by a computer-controlled, Stark modulated spectrometer in the frequency range 26 500 to 40 000 MHz, with a few spectra in the range 18 000 to 26 500 MHz. Measurements of absorption frequency, peak intensity, and integrated intensity are included along with experimental conditions, such as Stark field intensity, sample temperature and pressure, and microwave power level.

This report describes the apparatus and procedures used and presents tables of spectral data for the following compounds: acetonitrile, ammonia, 3-butenitrile, carbon oxide sulfide, dimethyl disulfide, ethanamine, ethanethiol, ethylene glycol cyclic sulfite, formamide, hydrocyanic acid, isoxazole, methanamine, methanethiol, methyl sulfide, methyl thiirane, nitroethane, nitromethane, propanenitrile, 2-propenenitrile, 2-propene-1-thiol, pyridine, pyrrole, sulfur dioxide, tetrahydrothiophene, thiazole, thietane, thiirane, and thiophene.

## INTRODUCTION

The potential of microwave spectroscopy as a method of chemical analysis has long been recognized. However, for many years the technique was not feasible because of the lack of suitable instrumentation and reference data. The first problem no longer exists, so that the major obstacle to the routine use of microwave analytical techniques is the lack of reference-data catalogs similar to those available in other wavelength regions. This report describes work at the Langley Research Center to compile such a catalog and presents some of the results.

The initial attempts at data compilation involved a survey of data from the scientific literature as well as measurements under contracts and university grants. Little useful data was found in the literature since most researchers confined their activities to searching for a few calculated absorption lines to verify molecular structures, so that most of the lines in the spectrum were never observed. Early attempts at the measurement of spectra specifically for analytical use were only partially successful because of the limita-

tions of the instrumentation then available. In 1966 a spectrometer which incorporated state-of-the-art microwave technology was procured, and some cataloging work was done at the Langley Research Center. However, the work proceeded slowly because of the large number of spectral lines encountered. Further, the sheer complexity of the instrumentation and amount of data handled resulted in an unacceptable level of operator errors and mistakes, such as transposition of digits.

It appeared that automation would be the only way to obtain the required quantities of data with a high degree of reliability, and cataloging efforts were therefore suspended until a computer-controlled system could be developed. Meanwhile, discussions with the National Bureau of Standards and other interested organizations were initiated, with the aim of coordinating efforts at reference-data compilation and setting standards for spectrometer performance and measurement accuracy (ref. 1).

Although most of the data presented in this report were obtained with the automated system, a few of the spectra were obtained with the manually controlled spectrometers. In the automated system, the spectrometer is operated and the data read out and processed by a dedicated digital computer. The final data are transferred via magnetic tape to the main computer center for printouts and punched cards, so that all chances for human error in data recording, computations, or key punching are eliminated. The data format used in the tables was developed in consultation with the Microwave Subcommittee of the Joint Committee on Atomic and Molecular Physical Data. A molecular frequency standard has been determined by the subcommittee and has been used to verify spectrometer accuracy for most of the data reported herein.

## SYMBOLS

$E_s$	intensity of Stark modulation square-wave electric field, kV/cm
$J$	angular momentum quantum number
$P$	microwave power at crystal detector, dBm
$p$	sample pressure, millitorr (1 torr = 133.3 N/m <sup>2</sup> )
$T$	sample cell temperature, K
$U$	frequency measurement uncertainty, MHz
$\gamma$	Beer's law absorption intensity coefficient, cm <sup>-1</sup>

$\Delta\nu$	half-width of absorption line at half-maximum-intensity point, kHz
$\nu_0$	frequency of absorption line at peak intensity, MHz

## APPARATUS

### Manually Controlled Spectrometers

The data in this report have been taken on one or more of three different spectrometers. The earliest measurements were performed with a Tracerlab model 4001KA, a 100-kHz Stark modulated spectrometer with stainless steel sample cells approximately 1 m long. The Stark electrodes were insulated by teflon slabs. Viton O-rings were used for the vacuum seals, and the vacuum system used an oil diffusion pump and a liquid-nitrogen cold trap. The microwave source was a phase-locked backward-wave oscillator which was stabilized by a resonant cavity. Direct frequency readout to 0.01 MHz was provided.

The measurements were later performed with a Hewlett-Packard model 8400B spectrometer. This instrument was similar to the one just described except for the addition of an arm to measure relative intensity, the use of a VHF oscillator to stabilize the microwave source, and the use of 33 kHz as the Stark modulation frequency. Other differences included a gold-plated sample cell and the use of an ion pump in the vacuum system. This spectrometer and its use have been described in reference 2.

### Automated Spectrometer

Except where otherwise specified, the data in this report were taken on the instrument described in the following paragraphs. This spectrometer is essentially a Hewlett-Packard model 8460A, adapted for computer control. It is different from the model 8400B primarily in the use of a digitally controlled reference oscillator which provides a resolution of 1 kHz in the range 18 000 to 40 000 MHz, and in the use of a longer sample cell (1.6 m). Operation from 18 000 to 26 500 MHz requires changing the microwave oscillator assembly and associated waveguide components, which cannot be accomplished on this system without letting the sample cell reach atmospheric pressure. Most of the data have therefore been taken in a single frequency range, and 26 500 to 40 000 MHz was selected since most molecules have more intense absorptions in this range.

Microwave source. - Figure 1 is a block diagram of the stabilized microwave source. The computer-source interface is a 44-bit output card. The first 32 bits are used to provide an 8-digit binary-coded decimal (BCD) frequency control word to the sweep control unit. This unit displays the requested frequency and programs the reference oscillator to a frequency between 400 to 420 MHz. The latter frequency is calculated to provide a

harmonic which is offset by the 20-MHz intermediate frequency from the final desired microwave frequency. The harmonics are generated by a snap-off diode and mixed with a sample of the microwave power. The backward-wave oscillator is pretuned to approximately the correct frequency by using the last 12 bits on the output card to program the helix voltage. The final tuning is done by a phase-error voltage from the synchronizer, which compares the intermediate frequency from the mixer with an internal 20-MHz oscillator.

Source output power is monitored by a thermistor-type power meter which can be monitored by the computer. In addition, a voltage output from the synchronizer indicates loss of lock. This output is monitored by the computer during measurement periods.

Modulation and detection.- Figure 2 illustrates the modulation, detection, and status monitoring system. The square-wave modulation voltage is programmable from 0 to 2000 V, base to peak, in 255 steps. Any deviation from the programmed voltage by more than a few volts, such as would occur from arcing in the cell or modulator malfunction, interrupts the computer and halts the program with an error message on the teleprinter. In addition to the square-wave amplitude control, the base voltage of the square wave is programmable in 255 steps over approximately a 10-V range to allow the baseline voltage to be set accurately to ground potential.

A signal at the 33-kHz modulation frequency is detected at the crystal detector, amplified by the tuned preamplifier, and sent to the phase-sensitive detector, where it is compared with a sample of the modulation frequency. The range setting of the phase-sensitive detector is programmable. However, the best results have been obtained by operating the detector on a fixed range setting and controlling the overall gain by an external precision VHF attenuator. This results in better linearity over a wide dynamic range and eliminates problems of baseline shifts with gain changes due to pickup in the detector of the modulation field.

The output of the phase-sensitive detector is measured by a voltage-to-frequency converter, which converts an input voltage into a series of pulses. These pulses are counted by an up-down counter during a precisely timed integration period. The specifications of the converter call for linearity within 0.01 percent of full scale, with overranging capabilities of 250 percent of full scale. This would provide a range of 0 to 250 000 counts per second. In practice, the converter has been observed to be linear to 350 000 counts per second. The combination of input voltage level and integration period must therefore be carefully chosen to avoid overflowing the input register on the counter, which can accept a maximum of 32 767 counts.

Status monitoring.- A second voltage-to-frequency converter is switched by a relay register to make a number of additional measurements. One of these is crystal current, which must be known accurately in order to calculate absorption intensities. Current is

measured with a precision of  $0.01\ \mu\text{A}$ , so that the limitation on repeatability is the temperature instability of the metering circuitry in the preamplifier.

Other measurements made for each spectral line include cell temperature, measured by a thermistor gage; sample pressure, measured by a capacitance manometer; and microwave power level at the crystal detector, sensed by another thermistor-type power meter. The power level was not controlled by the computer, but was kept within a narrow range by making frequent checks of crystal current. Whenever these checks showed that the current had reached programmed upper or lower limits, the scan was halted and the computer printed a request for a power-attenuator change on the teleprinter and sounded an alarm to attract operator attention.

Other status measurements have been previously mentioned. One is the phase-lock monitor, which is in use at all times when measurements are being made and during search operations. No discrete measurements are made on the modulators during normal operation, since the fault indicator is connected to the priority interrupt system, so that in effect the modulators are continuously monitored.

The capability for other measurements, such as phase-error voltage, exists but is used only during system checks or adjustments and is not part of the cataloging software.

Computer and peripheral equipment. - The spectrometer is controlled by a dedicated computer which has a core storage of 16 384 sixteen-bit words and a memory cycle time of  $1.6\ \mu\text{sec}$ . Two channels of direct memory access and a 184 000-word disc memory provide additional storage for data and for the system software, including test and calibration programs. Other peripheral equipment includes a teleprinter, photoelectric punched-tape reader, high-speed tape punch, oscilloscope-type XY-display, and magnetic tape recorder. Interfacing with the various spectrometer components is handled by plug-in circuit boards. Two crystal-controlled time-base generators provide for timing of integration periods and operation of a time-of-day clock. Figure 3 is a photograph of the computer and spectrometer system, taken before addition of the intensity calibration arm.

Calibration. - A BASIC language program is regularly run to provide a complete system checkout, including adjustment of the zero settings and sensitivities of the voltage-to-frequency converters, pressure gage, and phase-sensitive detector. A variable calibration signal is provided by the arm shown in figure 2. The arm is usable in the region from 26 500 to 40 000 MHz and is a recent addition. It was originally installed on the model 8400B spectrometer, and its use has been described in detail in reference 2. Sensitivity and linearity tests are made from one to three times daily with this bridge.

Sample and vacuum system. - Vacuum is provided by an ion pump and liquid-nitrogen cold trap. To improve the vacuum properties of the cell, seals were made by indium wire gaskets placed on the flat surfaces of the flanges between the O-ring grooves and the wave-

guide interior. This modification prevents the slow diffusion of gas into or out of the O-ring grooves and eliminates the necessity for exposing rubber and stopcock grease to the sample; thus, pressure stability is greatly improved.

The entire sample system is metal except for a fused-quartz bulb in which samples are frozen after injection, and some Kel-F and teflon seals in valves and fittings. The injection port contains a silicone rubber septum, but this is exposed to the system only at the time of sample injection and is then isolated from the system by a valve.

## SOFTWARE

The main control program is written in BASIC language. A driver routine for each instrument or component is written in assembly language, and these routines are called as subroutines from the main control program. One routine operates a time-base generator to provide time-of-day information to the program.

To begin operation, the control program requests parameters for the run, including frequency range to be covered, maximum gain setting to be used, power attenuator setting, and starting address to store data on the disc. The modulation voltage is set to 1000 V for the scan, and the gain is set to maximum. The scan then begins at the lower end of the programmed frequency range. A 30-msec detector time constant is used. During the scan, the crystal current is checked frequently. If it goes below 5  $\mu\text{A}$  or above 10  $\mu\text{A}$ , the scan is halted, and an attenuator setting is requested to bring the current back into the desired range.

When a signal above the threshold level of about one-third the full-scale value is detected, the program switches to a peak detection mode and brackets the line peak in successively smaller steps. The gain is adjusted as necessary during this operation to keep the signal near the full-scale value. After the frequency is set at approximately the line peak, the Stark baseline voltage is offset by about 0.5 V to check for a sensitive Stark effect. If this change produces a signal decrease of 1 percent or greater, the baseline voltage is adjusted to give maximum signal. Otherwise, it is reset to its initial value, and the square-wave voltage is then varied in 200-V increments to find the value which gives maximum signal. The program is written so that it gives preference to the 1000-V value and changes it only if necessary to give a better signal. This was found to be necessary because the clamping diodes in the modulator tend to heat and cool with large voltage changes and thus produce a slow drift of baseline voltage. On lines with sensitive Stark effects, this drift results in the development of zero basing errors after the measurement has started; consequently, the lines are broadened and the peak intensities reduced.



After the Stark field and the gain have been properly adjusted, a series of sweeps back and forth across the line begin. A 60-point array is used, and a running average of the signal at each point is kept. This is displayed on the oscilloscope screen, which allows observation of the signal-to-noise ratio and line shape. A variable-width scan is used to give the best signal-to-noise ratio at the line center, where it is most critical. Each pair of up-down sweeps is reduced in width until only the middle third of the array is being scanned. The entire cycle then repeats by beginning with a full 60-point scan. The total number of sweeps required is calculated as a function of gain setting. When the signal averaging is completed, the signal-to-noise ratio is further improved by 11-point cubic smoothing.

The five points at each end of the array are not used since the digital filtering is not symmetric for them. This leaves 50 data points across the spectral line. The frequency step size used in scanning is such that both the half-maximum-intensity points are included, with the further constraint that there must be at least 20 points between the 2 half-maximum points. If either of these conditions is not met, the program calculates a new step size which will meet them and repeats the scan. However, logic is included to recognize overlap situations to prevent the step size from being increased to include several overlapping lines. The program is also satisfied to measure only one of the half-widths of a line which is asymmetric because of unresolved fine structure or overlaps, since width data are of little value in such a case.

After the final smoothed data array has been obtained, the spectral parameters are calculated. The resonant frequency is found by using linear interpolation between the data points to find the value at which the first derivative of the line shape is zero. This method was found to be accurate to 1 kHz with as few as 10 data points. The maximum measured signal value from the smoothed array is used to calculate the absorption coefficient, with the integration period, gain setting, and crystal current taken into account. Further interpolations are then done to find the frequencies corresponding to the half-maximum-intensity points on either side of the array. The average value of the half-widths is used to provide a measure of the integrated intensity. Any asymmetry noted is used as one of the criteria in determining the estimated frequency uncertainty for the measurement.

All spectral data which will go into the catalog are stored on the disc. They are also printed on the teleprinter along with other experimental conditions, such as gain setting, frequency step size used, and time of day. The scan then resumes from the peak of the line. As the signal decreases, the gain is increased back to the maximum value. At that point, after the signal drops below the threshold level, the normal search mode is resumed. However, if a signal increase is noted at any time during this operation, the program reverts to the peak detection mode and prepares to measure the new line. This

program has successfully been used to measure overlapping lines with an apparent peak separation of less than 0.25 MHz.

## EXPERIMENTAL PROCEDURES

### Samples

All samples except hydrogen cyanide were commercially available reagents or bottled gases. Each was analyzed for impurities on a chromatograph with porous polymer columns and a dual thermal-conductivity detector. In most cases the impurities were small (a few tenths of 1 percent or less) or could be reduced by vacuum distillation in the sample manifold. When necessary, the samples were chromatographically purified.

Samples were injected through a silicone rubber septum into the manifold, and the septum was then shut off from the system. The samples were frozen at liquid nitrogen temperature in a small fused-quartz bulb, and any remaining air was then pumped off. The temperature was adjusted as necessary to allow pumping off of volatile impurities or to allow admission of sample vapors to the cell while less volatile impurities were kept frozen. Procedures were similar for the chromatographically purified samples, except that they were not injected through the septum. Instead, the effluent from the chromatograph was trapped in a small stainless steel trap which was connected directly to a fitting on the sample manifold.

Sample pressures were usually 10 to 20 millitorr. The pressure was chosen to be as high as practical in order to minimize pressure measurement errors and the effects of slight leaks, adsorption, and desorption. The higher pressures also minimized effects of power saturation. The upper limit on pressure was determined by the line widths. Values of 200 to 300 kHz were preferred in order to provide good accuracy and resolution in frequency measurements and to insure that complete Stark modulation could be achieved. Some samples, particularly those containing nitrogen, had line widths of 500 kHz or greater even at reduced pressures, and these were run at pressures below 10 millitorr.

### Spectral Measurements

The measurement process was completely automated with no opportunity for operator intervention except for the option of interrupting, and thus terminating, a run at any time. Each spectrum was run in several portions to allow a periodic test of sample purity and spectrometer performance. This test consisted of remeasuring the first line detected on each run to check for agreement of intensities and line widths. If a change was noted, the sample was pumped out and the pressure gage zero and the system were checked. In the event that the system calibration had drifted as a result of temperature changes, the new calibration was added to the program before the run was continued. When a change was

attributed to leaks or sample degradation, a fresh sample was added and thereafter the sample was changed frequently enough to keep intensity variations to about 5 percent or less.

After the complete spectrum was obtained, a fresh sample was added and a few of the stronger lines from each run were remeasured to check for calibration and sample consistency between the various runs.

Two other checks on the data were available for many of the samples. One was a comparison with data from the earlier work with the two manual spectrometers. Data from those instruments ranged from actual frequency and intensity measurements to strip-chart recordings of the spectrum. In any case, they provided a further check on the consistency of the observed spectra on various instruments and samples. A final verification that the spectra did indeed belong to the molecules to which they were attributed was made whenever possible by the assignment of some of the observed lines to specific rotational transitions of the molecules. The procedures used are noted in each case in the discussion preceding the table.

### Data Processing

All spectral parameters and measurement conditions were in final form when stored on the disc. It was usually necessary only to run a FORTRAN program to transfer these data to magnetic tape in BCD format. The tape was then sent to the main Langley Computer Complex, where listings were printed and cards were punched under computer control. The card decks were used to produce the tables in this report.

On some occasions slow steady changes in peak and/or integrated intensities were noted. These were usually caused by drift in the spectrometer calibration or the zero setting of the pressure gage as the laboratory temperature varied. Occasionally they were caused by sample degradation. In most cases, it was possible to use the time-of-day information printed with each measurement to establish a drift rate and correct the data. It was experimentally determined that this method of correction was accurate to within 0.1 dB in most cases. The correction was therefore applied to some of the stronger lines in those spectra where drift was noted and where the intensity measurement accuracy justified keeping a resolution of 0.1 dB. This type of data manipulation was done as sparingly as possible since it partially defeated the advantages in reliability of having a completely automated operation.

### EXPLANATION OF THE TABLES

#### Names

Spectral data are tabulated alphabetically by molecule name in the section entitled "Spectral Tables." The naming system is that used by Chemical Abstracts, volume 76,

1972. When a molecule is more commonly known by another name or names, these are also listed and a cross reference is inserted in the index to the tables. In addition to the name or names, the discussion before each table also includes the formula and the Chemical Abstracts Service (CAS) Registry number for further identification.

A second molecule identification number is given for the sake of completeness. This number is part of an internal system developed by the National Bureau of Standards for computer handling of spectral data to be published in supplements to Monograph 70 (ref. 3). It is also used for computer handling of data at the Langley Research Center.

#### Sample and Remarks

The discussion preceding each table gives the sample source and the results of a chromatographic purity check along with details of any further purification done. Also given are pertinent remarks on experimental conditions or results, including the availability of other experimental or theoretical data to verify sample identity.

#### Frequency Data

The first two columns of each table give the peak frequency, listed in increasing order, and the measurement uncertainty, both in MHz. The spectrometer frequency is standardized at the value for the  $J = 2 \rightarrow 3$  transition of the main isotope of carbon oxide sulfide. In measurements made by LeRoy Scharpen, of the Hewlett-Packard Company, under the auspices of the Joint Committee on Atomic and Molecular Physical Data, this line was found to have a frequency of  $36\,488.8118 \pm 0.0003$  MHz at a pressure of 5.5 millitorr. This measurement was made by using radio station WWV as a standard. It should be noted that this value was not obtained until late 1972 and could not be applied to the data taken earlier in the range 18 000 to 26 500 MHz.

The measurements made by the automated system are given to 0.001 MHz unless the uncertainty is 0.1 MHz or more, in which case they are rounded to the nearest 0.01 MHz. The uncertainties are usually much larger than the actual experimental errors. The value calculated by the computer is based on line width, the frequency step size used, asymmetry of the line if any, intensity of the line, and the sensitivity of the Stark effect. The tabulated uncertainty is the first value equal to or greater than the calculated value from the sequence 0.01, 0.02, 0.05, 0.1, 0.2 MHz.

#### Intensity Data

The third column of the tables gives the peak relative intensity in the form  $-10 \log (\gamma_1/\gamma_2)$ , where  $\gamma$  is the Beer's law absorption coefficient in  $\text{cm}^{-1}$ . For convenience the reference value  $\gamma_2$  is chosen to be unity, so that the tabulated intensities are numerically

equal to  $-10$  times the logarithm of the absolute intensities. The latter notation is used in the tables. The logarithmic form was chosen in the discussions mentioned in the Introduction as being the most efficient way to catalog numbers which varied over many orders of magnitude. A further advantage is that the calculation of intensities from manually operated spectrometers is simplified, since most meters and attenuators are calibrated in decibels. This point is discussed in detail in reference 2.

The earlier intensity measurements were relative to a molecular standard. A value of  $\gamma = 1.9 \times 10^{-4} \text{ cm}^{-1}$  for the  $J = 2 \rightarrow 3$  transition of carbon oxide sulfide was used (ref. 4). Later the calibration arm shown in figure 2 was added and is used for daily checks of calibration and linearity. The arm is calibrated by an absolute technique in which the modulation sensitivity of the source is measured, and a known value of  $\Delta P/P$  is then produced by modulating the source with a sample of the Stark modulation voltage. The characteristics of the crystal detector are also calibrated by using a constant value of  $\Delta P/P$  over the range of currents to be used. Polynomials are then found which will reproduce these characteristics within 1 percent. These polynomials are used during spectral measurements to compensate for variations in sensitivity due to operation at different values of current than the one used for initial calibration. This procedure was used only above 26 500 MHz, which is the lowest frequency for operation of the calibration arm.

Measurements were made below 26 500 MHz during a brief period early in the development stage only, and no separate calibration was done to adjust for the characteristics of the detector in the low range. The same calibration, based on the carbon oxide sulfide measurements, was used. Intensity measurements in this range are therefore likely to have considerably larger errors.

Most of the intensity measurements are given to the nearest decibel. Many of the stronger lines measured since installation of the calibration arm are given to 0.1 dB. These measurements are generally repeatable within 0.3 dB from time to time, although the absolute accuracy may be somewhat less. Intensities in the range below 26 500 MHz may be in error by 1 to 2 dB. Aside from the inaccurate calibration, other reasons for rounding intensities to the nearest decibel include low intensities, where noise or stray pickup can cause larger errors; sensitive Stark effect, which could result in broader and weaker lines if the modulator zero base is imperfect; and overlap or unresolved fine structure, which distorts the line shape and causes the observed frequency and/or intensity to vary with pressure.

The fourth column of the tables gives the integrated intensity per unit of pressure in the form  $-10 \log(\gamma \Delta\nu/p)$ , where  $\Delta\nu$  is the line half-width in kHz and  $p$  is the sample pressure in millitorr. This is also a relative measurement, with the reference value of  $\gamma \Delta\nu/p$  taken as unity. The rounding conventions are the same as for the peak intensity.

The values given only to the nearest decibel should not be relied on for quantitative measurements, since they may not be constant with pressure variations, in the case of asymmetric lines. In many such cases, only one of the half-widths was measured, and the value of  $\gamma\Delta\nu$  will not be the same as it would for a measurement where  $\Delta\nu$  was taken as one-half the total width.

### Line-Type Classification Code

For all lines where some information is missing or rounded off, a code number is given in the column "Line-Type Code" to indicate the reason. The code is defined in table 1. In the event that more than one of the code numbers is applicable, the lower one takes priority.

TABLE 1.- DEFINITION OF LINE-TYPE CODE

<u>Code</u>	<u>Meaning</u>
1	No line width data available; line is unusually broad (e.g., the center line of a partially resolved triplet), or data were taken before line width measurements were routinely made
2	Only upper half-width measured; lower half-width is greater and did not fall inside data array; the frequency and/or intensity may be pressure dependent
3	Only lower half-width measured; upper half-width is greater; same significance as type 2
4	Asymmetric line; both widths measured but they differ by at least 5 percent; same significance as types 2 and 3
5	Low intensity: $-10 \log \gamma$ is more than 60.5
6	Sensitive Stark effect; modulator zero field errors may cause broadening, weakening, or shift
7	Incomplete or lower quality data; taken manually or during early automation development; often refers to other than intensity data

The following procedures were used to find the integrated intensity: For any line where both half-widths were measured, the average of the two was used. For type 2 lines, the integrated intensity is based on only the upper half-width; for type 3 lines, the lower half-width. Note that the only significant difference between these lines and a type 4 (asymmetric) line is that the step size was large enough to cover both half-maximum-intensity points for type 4, but not for the others. This seems to imply greater asymmetry for types 2 and 3, but that is not always the case. Since the program will not remeasure an asymmetric line merely to obtain the second half-width, whether a line is

classified as type 2, 3, or 4 sometimes depends only on the circumstantial relationship between line width and the initial frequency step size used.

### Stark Field

The tabulated intensity of the Stark modulation field is the value at which the measurements were made, and is usually the value which gave the best signal. Allowable values of voltage were 800 to 1800 V in 200-V increments for the automated system. Any significant undermodulation or interference is readily detected since signal variations of 0.5 percent or greater are considered.

Each line is tested for sensitivity of Stark effect by offsetting the zero field voltage from ground potential by about 0.5 V. If a signal loss of 1 percent or more is noted, the line is classified as sensitive, and the field value is followed by S in the tables. This indicator does not apply to lines below 26 500 MHz in frequency, since these were run at an early stage of software development when information on Stark sensitivity was not included in the data output.

### Power

The power  $P$  given in the seventh column is that measured at the detector. The input power to the cell is greater by about 1 to 2 dB, depending on frequency. The power levels were not measured during operation below 26 500 MHz.

### Temperature

The absolute temperature of the sample cell as measured by a thermistor-type gage is given in the eighth column. All the measurements were made at ambient room temperature; therefore, the maximum temperature variation was about 8 K.

### Pressure

The ninth column gives the sample pressure. Tabulated values are the absolute measurements made with a capacitance manometer. In many cases the pressure was also measured by a thermocouple gage, and this information is given in the discussions preceding the tables. Depending on sample composition, the thermocouple measurements may give readings up to 300 percent greater than the absolute measurements.

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Methyl mercaptan, see Methanethiol	
Methyl sulfide . . . . .	55
Methyl thiirane . . . . .	60
Methylthiomethane, see Methyl sulfide	
Nitroethane . . . . .	62
Nitromethane . . . . .	64
Propanenitrile . . . . .	67
2-Propenenitrile . . . . .	69
2-Propene-1-thiol . . . . .	72
Propionitrile, see Propanenitrile	
Propylene sulfide, see Methyl thiirane	
Prussic acid, see Hydrocyanic acid	
Pyridine . . . . .	74
Pyrrole . . . . .	80
Sulfur dioxide . . . . .	85
Tetrahydrothiophene . . . . .	87
Thiazole . . . . .	90
Thietane . . . . .	92
Thiirane . . . . .	97
Thiofuran, see Thiophene	

Thiophene . . . . .	99
Trimethylene sulfide, see Thietane	
Vinyl cyanide, see 2-Propenenitrile	

### Acetonitrile

Formula:  $\text{CH}_3\text{CN}$

CAS Registry number: 75-05-8

Synonyms: methyl cyanide, ethanenitrile

NBS identification number: 151.00

Frequency range: 18 000 to 40 000 MHz

Sample.- The sample was Fisher A-24 Certified reagent. Chromatography on a Chromosorb 102 column showed only a water impurity of less than 0.5 percent. This was minimized by distilling the acetonitrile into the cell at low temperature.

Remarks.- These lines are exceptionally broad, and the fine-structure components are resolved only at low pressure. Because of the amount of overlap, the intensities and frequencies of most of the lines are quite pressure dependent.

Most of the lines have been verified theoretically (ref. 3). In addition, data were available from work performed under NASA contract and from measurements on the Tracerlab spectrometer above 26 500 MHz. Data below 26 500 MHz include no information on Stark sensitivity or power levels. The power was generally below -15 dBm.

NAME: ACETONITRILE						ID NO. 151.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
18396.76	.10	59	40	3	2.1		299	4
18398.02	.02	56	37	7	2.1		299	4
18399.90	.10	63	44	2	2.1		299	4
18451.82	.05	66	47	4	2.1		299	4
18453.09	.02	64	45	7	2.1		299	4
35688.04	.05	70	50	4	2.6		299	3
35732.03	.20	69	48	3	3.0		299	3
35733.18	.05	66	46	4	3.0		299	3
36610.49	.05	65	45	4	1.7		299	3
36773.57	.10	68	47	4	1.7		299	3
36776.18	.20	69		1	1.7		299	3
36777.24	.05	66	45	4	2.1		299	3
36794.37	.10	48	26	3	1.7	-17	297	3
36795.536	.02	44	24	4	1.7	-17	297	3
36797.588	.02	53	33	4	2.1	-17	297	3
36869.82	.10	58	39	3	3.0	-17	297	3
36871.13	.10	56	35	4	3.0S	-17	297	3
36902.27	.10	60	40	3	2.6S	-17	297	3
36903.63	.10	57	33	3	2.6S	-17	297	3
36904.34	.10	57		1	1.7	-17	297	3
36905.636	.02	52.5	33.4		1.7	-17	297	3
36907.69	.05	62	42	4	1.7		297	3
36940.98	.10	58	39	3	2.1S	-17	297	3
36941.60	.10	59		1	1.7		297	3
36942.29	.10	56	36	4	2.1S	-17	297	3
37010.52	.20	63		1	2.1		297	3
37011.797	.05	59	39	2	1.7	-17	297	3
37013.614	.02	60	41	4	1.7	-17	297	3

## Ammonia

Formula:  $\text{NH}_3$

CAS Registry number: 7664-41-7

NBS identification number: 173:00

Frequency range: 18 900 to 40 000 MHz

Sample.- The sample was Matheson anhydrous grade bottled gas with a stated purity of 99.99 percent. No impurities were detected by chromatography with a Chromosorb 102 column.

Remarks.- Ammonia was strongly adsorbed and it was necessary to add sample to the cell periodically to maintain the desired pressure.

The shapes of many of the stronger lines are distorted by unresolved or partially resolved fine structure; thus, the lines are unsuitable for quantitative use unless individual calibration curves are obtained for all line widths which may occur.

The sample identity was confirmed by matching most of the lines with theoretical transitions (ref. 3).

Data below 26 500 MHz contain no information about Stark sensitivity or power levels. However, the power was generally less than -15 dBm.

NAME: AMMONIA					ID NO. 173.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
18017.33	.02	45	33	7	2.1		298	8
18127.10	.02	54	41	7	2.1		298	8
18162.35	.02	54	41	7	2.1		298	8
18285.43	.02	51	38	7	2.1		298	8
18391.48	.05	56	42	4	2.1		298	7
18499.39	.02	46	33	7	2.1		298	9
18808.50	.02	47	34	7	2.1		299	9
18884.70	.02	48	37	7	2.1		299	9
19218.46	.02	46	33	7	2.1		299	8
19757.56	.05	42	29	4	2.1		299	9
20371.45	.02	45	33	7	2.1		299	9
19838.39	.05	52	39	4	2.1		299	9
20719.22	.02	41	28	7	2.1		299	9
20735.45	.02	46	33	7	2.1		299	9
20804.85	.05	43	30	4	1.7		299	9
20852.53	.02	50	37	7	2.1		299	9
20994.63	.02	41	28	7	2.1		299	8
21070.74	.02	48	34	7	1.7		299	9
21134.30	.05	48	35	4	2.6		299	8
21285.28	.02	38	24	7	2.1		299	9
21391.62	.02	53	40	7	2.1		299	10
21637.90	.02	60	46	7	2.1		299	9
21703.36	.02	41	29	7	2.1		299	9
21817.98	.02	57	43	7	2.1		299	9
21846.41	.02	62	48	7	2.1		299	9
22233.21	.20	58	43	3	3.4		299	9
22233.46	.20	58		1	3.8		299	8
22234.50	.05	46	33	4	3.0		299	8
22353.91	.02	59	44	7	2.1		299	8
22649.86	.20	59	43	3	2.1		299	8
22653.02	.02	39	25	7	2.1		299	8
22688.31	.02	36	23	7	1.7		299	9
22732.43	.02	39	25	7	1.7		299	9
22789.43	.02	59	45	7	1.7		299	9
22834.19	.05	39	26	4	2.1		299	9
22924.94	.02	37	23	7	2.1		299	9
23097.84	.20	53	39	3	2.1		299	8
23098.16	.20	52		1	2.1		299	8
23098.82	.02	42	30	7	2.1		299	8
23099.48	.20	52		1	2.1		299	8
23099.79	.20	53	39	2	2.1		299	8
23232.23	.02	41	28	7	2.1		299	9
23421.98	.02	61	47	7	2.1		299	9
23657.47	.02	43	29	7	2.1		299	9
23692.97	.10	48	33	4	2.1		299	9
23693.93	.10	46	31	3	2.6		299	9
23694.49	.02	42	28	7	2.1		299	9
23695.07	.10	46	32	2	2.6		298	9
23696.03	.10	48	34	4	2.1		298	9
23720.60	.20	49	35	3	2.1		298	9

NAME: AMMONIA			CONTINUED			ID NO. 173.00		
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
23721.36	.20	48		1	3.4		298	9
23722.64	.02	37	23	7	2.1		298	9
23723.92	.20	48		1	3.4		298	9
23724.69	.20	48	33	2	3.0		298	9
23867.83	.20	47	32	3	2.1		298	9
23868.46	.20	46		1	2.1		298	9
23870.13	.02	34	19	7	2.1		298	9
23871.79	.20	47		1	2.1		298	9
23872.44	.20	48	33	2	2.1		298	8
24136.96	.20	51	36	3	1.7		298	9
24137.51	.20	51		1	2.1		298	9
24139.42	.02	36	21	7	2.1		298	9
24141.32	.20	51		1	2.6		298	9
24141.87	.20	52	36	2	2.6		298	9
24205.29	.02	43	29	7	2.1		298	9
24530.43	.20	52	36	3	2.6		298	9
24530.90	.20	52		1	2.1		298	9
24532.99	.02	36	22	7	2.1		298	9
25053.39	.20	52	35	3	2.1		298	9
24881.92	.02	48	35	7	2.1		298	9
25053.82	.20	51		1	2.1		298	9
25056.02	.02	34	20	7	2.1		298	9
25695.23	.02	52	38	7	2.1		296	8
25715.18	.02	38	23	7	2.1		296	8
26518.987	.02	36.5	22.0		2.1	-18	298	10
26654.853	.01	49	34	4	1.7	-18	298	10
27477.932	.01	35	21	4	2.1	-18	298	10
27772.295	.02	55	41	4	2.1	-18	298	10
28604.739	.01	40.0	25.6		2.1	-18	298	10
29061.192	.01	57.9	43.9		2.1	-17	298	10
29914.487	.01	42.2	27.8		2.1	-17	298	10
30537.408	.02	59	44	4	2.1	-17	298	10
31424.945	.01	41.7	27.3		2.1	-16	298	10
32036.631	.02	62.5	48.1		2.1	-16	298	10
32110.768	.05	65	50	4	2.1	-16	298	10
33156.857	.01	47.1	32.8		2.1	-16	298	10
35134.307	.01	50.2	35.7		2.1	-16	298	10
37385.138	.01	50.1	35.6		2.1	-16	298	10
39941.422	.01	56.6	42.1		2.1	-16	298	10

### 3-Butenenitrile

Formula:  $\text{CH}_2\text{:CHCH}_2\text{CN}$

CAS Registry number: 109-75-1

Synonyms: allyl cyanide, vinyl acetonitrile

NBS identification number: 767.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample source was Eastman 3182. Gas chromatography with a Chromosorb 102 column showed only a single impurity peak of less than 0.1 percent, which was tentatively identified as water.

Remarks.- The lines are exceptionally broad and many of the widths were not measured at a pressure of 10 millitorr. Those that were measured ranged from 0.75 to near 1 MHz, and most were asymmetric because of the fine structure. Many of the stronger lines were remeasured at a pressure of 5 millitorr. The frequencies and intensities of many of the lines were pressure sensitive because of the asymmetry.

The sample pressure of 10 millitorr was registered by a thermocouple gage as 36 millitorr, and the pressure of 5 millitorr was registered as 18 millitorr.

NAME: 3-BUTENENITRILE							ID NO. 767.00	
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
27995.82	.20	66	47	2	3.4	-17	296	10
28085.785	.05	65	46	4	3.8	-17	296	10
30331.488	.02	65	46	5	3.4	-18	296	5
30380.840	.02	64	45	5	3.0	-17	296	5
30406.82	.20	65	45	2	3.8	-17	297	10
30506.830	.05	64	46	5	2.1S	-17	296	5
30679.57	.20	64	45	2	3.4	-17	297	10
30703.30	.20	64	45	2	3.0	-18	296	10
30714.84	.10	63	42	4	2.1S	-18	298	5
30720.30	.10	63		1	2.1S	-17	296	10
30726.364	.02	65	45	5	2.6	-18	298	5
30728.30	.10	65		1	2.6S	-18	297	10
30800.69	.20	65	46	5	2.1S	-18	297	10
30832.936	.02	64	44	4	3.0	-17	297	5
30876.821	.02	65	46	5	3.0	-18	297	5
31064.994	.02	65	46	5	3.0	-18	297	10
31668.731	.05	64	45	4	2.1	-18	297	5
32093.536	.02	65	46	5	2.1	-19	297	5
32396.640	.02	63	45	5	2.1	-18	297	10
32693.937	.02	65	46	5	3.8	-17	297	10
32828.033	.02	64	45	5	2.6	-17	297	10
32845.00	.20	65	45	2	2.1	-18	297	10
33201.39	.10	66		1	2.1	-15	297	10
33278.34	.10	65		1	2.1	-17	297	10
33747.477	.02	65	46	5	1.7	-16	296	10
34145.941	.02	64	45	5	3.0	-17	296	5
34506.736	.05	65	47	4	3.4	-16	296	10
34822.559	.02	62	43	4	2.1	-18	296	5
35004.33	.20	66	47	3	2.1	-16	296	10
35171.047	.02	62	44	5	2.6	-17	297	10
35383.727	.02	63	44	4	3.4	-17	296	5
35471.57	.10	65	48	4	3.4S	-17	297	10
35781.11	.20	65	46	3	3.4	-17	296	5
35782.363	.02	62	43	4	3.0	-16	296	5
35818.304	.05	63	43	4	3.4	-17	296	5
35834.53	.10	60	40	6	3.8S	-16	296	5
35840.31	.20	61	41	4	3.0S	-16	296	5
35849.64	.10	61		1	2.6S	-16	297	10
35854.92	.20	62	43	2	3.4	-16	298	10
35861.53	.10	65		1	3.8S	-16	298	10
35880.272	.05	63	44	4	2.1	-16	298	10
35917.847	.05	64	45	4	3.4	-16	298	10
35934.79	.20	62	43	4	3.0S	-16	298	10
35940.54	.20	63	44	2	3.0S	-16	298	10
35950.08	.10	65		1	2.1S	-16	298	10
35955.23	.10	64		1	3.4S	-16	298	10
35962.85	.20	64	44	2	3.8	-16	298	10
36020.10	.20	65	46	4	3.4S	-16	298	10
36026.34	.20	65	46	3	3.8S	-17	298	10
36094.34	.10	65		1	3.0	-16	298	10



NAME: 3-BUTENENITRILE

CONTINUED

ID NO. 767.00

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
36239.219	.02	63	45	5	3.8	-16	298	10
36349.87	.10	65	47	5	3.0S	-16	298	10
36408.216	.05	65	47	4	2.1	-16	296	10
36436.752	.05	65	46	5	3.0	-16	296	10
36460.522	.05	62	43	4	1.7	-16	296	10
37211.70	.10	65		1	2.1	-17	296	10
37406.39	.20	64	45	2	3.4	-15	295	10
37451.828	.05	65	46	4	1.7	-16	295	10
37459.818	.05	61	42	5	2.1	-16	296	10
38232.724	.05	63	44	4	3.0	-16	296	10
38243.032	.05	65	46	4	3.0	-16	296	10
38694.131	.05	65	46	4	3.0	-16	296	10
39132.017	.05	64	45	4	1.7	-15	296	10
39179.000	.02	62	43	5	3.8	-15	296	10
39261.777	.05	62	43	4	1.7	-15	296	10
39271.44	.10	65	47	4	3.0S	-15	296	10
39656.682	.05	65	46	4	3.4	-14	296	10
39771.43	.20	63	44	5	3.0S	-15	296	10
39796.23	.10	63		1	3.8	-15	297	10
39832.36	.20	64		1	3.4S	-15	297	10
39833.39	.10	65		1	3.8	-15	297	10
39837.58	.20	65		1	3.8S	-15	297	10
39888.27	.20	62	43	3	3.0	-15	297	10
39916.98	.20	64	45	2	2.6	-15	297	10

## Carbon oxide sulfide

Formula: OCS

CAS Registry number: 463-58-1

Synonyms: carbonyl sulfide, carbon oxysulfide

NBS identification number: 130.00

Frequency range: 18 000 to 40 000 MHz

Sample.- The sample was Matheson bottled gas with a stated purity of 97.5 percent. Chromatography on a Chromosorb 102 column showed an impurity peak of about 2 percent which could not be positively identified but may have been air. One sample was chromatographically purified, but the measured intensities did not differ significantly from other samples.

Remarks.- The spectrum of carbon oxide sulfide has been extensively studied and all the lines have been theoretically verified (refs. 3 and 4). The 36 488.812 MHz line is used as a frequency standard. For this purpose the pressure should not exceed about 20 millitorr, because incomplete Stark modulation at the higher pressures causes an apparent upward frequency shift.

Data from 18 000 to 26 500 MHz include no information on Stark sensitivity or power level. However, power levels were generally less than -15 dBm.

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
35596.873	.01	51.0	43.0	6	3.8	-18	293	25
36371.405	.01	56.8	48.7		3.8	-18	293	25
36380.002	.01	55.6	47.5		3.8	-17	293	25
36488.812	.01	37.0	28.9		3.8	-17	293	25
36533.252	.01	49.0	40.8		3.4	-18	293	25
36571.423	.01	48.9	40.7		3.4	-18	293	25
36601.030	.01	59.7	51.8		3.4	-17	293	25
36615.267	.05	59	51		2.15	-18	293	25

## Dimethyl disulfide

Formula:  $\text{CH}_3\text{SSCH}_3$

CAS Registry number: 624-92-0

Synonyms: methyl disulfide, methyldithiomethane

NBS identification number: 328.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample source was Aldrich 15,031-2, with the identity confirmed by the manufacturer by gas chromatography and infrared analysis. Chromatography on a Chromosorb 102 column showed only two impurities of less than 0.1 percent each.

Remarks.- Some of the lines were also measured at a pressure of 10 millitorr, but the intensities are at the threshold level and not all lines were detected at the lower pressure. At 10 millitorr, a thermocouple gage registered a pressure of 32 millitorr.

NAME: DIMETHYL DISULFIDE					ID NO. 328.00			
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
27513.211	.02	65	50	5	2.1	-20	296	15
27785.70	.20	66	51	2	2.6	-18	296	15
27923.64	.10	65		1	3.0	-18	297	15
32108.913	.02	65	50	5	2.1	-16	297	15
33906.966	.05	63	47	4	3.8	-16	297	14
34014.852	.05	66	49	5	2.1	-16	297	15
34440.86	.20	64	49	2	3.0	-16	297	15
34731.111	.02	63	48	5	2.1	-16	298	15
36287.002	.02	65	50	5	2.1	-14	298	15
36482.399	.02	65	49	5	2.6	-14	298	15
36644.750	.02	63	48	5	3.0	-15	298	15
39182.615	.02	63	48	5	3.0	-15	298	15

## Ethanamine

Formula:  $\text{CH}_3\text{CH}_2\text{NH}_2$

CAS Registry number: 75-04-7

Synonyms: ethylamine, aminoethane

NBS identification number: 329.00

Frequency range: 26 500 to 40 000 MHz

Sample. - The sample was Eastman P506, a 70 percent aqueous solution. The sample was frozen at liquid nitrogen temperature and then warmed just sufficiently to admit ethanamine to the cell. Ammonia lines were monitored during the run, and the maximum concentration observed at any time was 0.5 percent.

Remarks. - Most of these lines show considerable asymmetry due to unresolved or partially resolved fine structure. Many of the components are sufficiently resolved to be measurable but were not detected since they were below the sensitivity limit.

Data were compared with a strip-chart recording of the spectrum run on the Tracer-lab spectrometer with 10-MHz frequency markers and with scans of some of the stronger lines run later on the Hewlett-Packard 8400B with 1-MHz markers.

NAME: ETHANAMINE					ID NO. 329.00			
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
26605.021	.05	61	47	4	2.1	-19	298	10
27127.50	.10	65	50	4	1.7	-19	298	10
27183.72	.10	64	50	4	1.7	-19	298	10
27550.194	.05	59	46	4	2.1	-19	298	10
27821.23	.10	64	50	3	2.1	-19	298	10
27891.49	.10	67	55	3	1.7	-18	297	10
28604.731	.02	64	51	5	1.7	-19	298	10
28619.033	.05	63	51	4	2.1	-19	298	10
28685.318	.05	64	52	3	2.0	-19	298	10
29016.470	.05	60	47	3	2.1	-17	298	10
29016.77	.10	61	48	2	2.1	-17	298	10
29893.567	.05	59	45	4	2.1	-18	298	10
30094.057	.05	61	48	3	2.1	-18	298	10
30390.584	.05	64	50	4	2.6	-17	298	10
30627.269	.05	64	51	4	2.6	-17	298	10
31508.620	.02	58	45	4	2.1	-18	298	10
31702.139	.02	63	51	5	2.1	-18	298	10
31783.43	.10	63	48	3	2.1	-17	298	10
31899.45	.10	64	52	3	1.7	-17	298	10
32295.169	.05	63	50	4	2.1	-18	298	10
32378.568	.05	60	46	4	2.1	-18	298	10
32651.92	.10	65	51	2	2.1	-17	298	10
32776.14	.10	65	53	3	2.1	-17	298	10
33067.412	.02	64	51	4	2.1	-18	298	10
33131.604	.05	59	44	4	2.6	-18	298	10
33228.545	.02	63	49	4	2.1	-18	298	10
33820.795	.05	59	46	3	2.1	-18	297	10
33821.14	.10	61	48	2	2.1	-18	297	10
34203.374	.02	63	50	5	3.0	-17	297	10
34527.390	.05	64	51	4	1.7	-17	297	10
34667.036	.05	59	46	3	2.1	-17	298	10
34912.941	.02	65	54	5	1.7	-17	298	10
34984.880	.02	63	49	4	2.1	-17	298	10
34985.36	.10	66	53	2	2.6	-17	298	10
35182.680	.02	64	51	5	2.1	-18	298	10
35299.796	.05	65	51	4	2.1	-18	298	10
36144.159	.02	62	49	4	2.1	-17	298	10
36171.312	.05	63	49	4	2.1	-17	298	10
36290.730	.05	63	50	4	2.1	-17	298	10
36373.02	.10	63	50	3	1.7	-17	298	10
36589.60	.10	63	51	3	2.1	-17	298	10
36589.95	.10	66	53	2	2.1	-17	298	10
36747.980	.05	59	46	4	2.1	-17	298	10
36750.48	.10	64	52	3	3.4	-17	298	10
37744.293	.05	64	50	4	2.1	-16	298	10
37781.662	.05	58	43	4	1.7	-18	299	10
38008.007	.02	65	52	4	3.0	-17	299	10
38476.868	.02	64	51	5	3.0	-17	299	10
38701.966	.05	58	46	3	2.1	-17	299	10
38702.35	.10	61	48	2	2.1	-17	299	10

NAME: ETHANAMINE			CONTINUED			ID NO. 329.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
38971.769	.05	58	45	4	2.1	-16	299	10
39077.935	.02	64	51	4	3.4	-17	299	10
39204.573	.05	64	50	4	2.1	-17	299	10
39271.210	.05	65	51	4	2.6	-17	299	10
39296.979	.05	57	45	3	2.1	-15	298	10
39429.144	.02	62	49	4	1.7	-16	298	10
39433.46	.10	63	51	3	2.6	-16	298	10
39519.467	.05	58	46	3	2.1	-16	298	10
39519.78	.10	61	48	2	2.1	-16	298	10



## Ethanethiol

Formula:  $\text{CH}_3\text{CH}_2\text{SH}$

CAS Registry number: 75-08-1

Synonym: ethyl mercaptan

NBS identification number: 327.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman 958. Chromatography on a Chromosorb 102 column showed one impurity of about 0.5 percent and one of less than 0.1 percent. Methanethiol was detected in the first sample, but after several distillations the amount remaining was barely detectable.

Remarks.- Only the doublet at 39 653 MHz was strong and symmetric enough for quantitative use, and overlap is a problem with it at pressures of 10 millitorr or greater.

The sample was not stable in the cell and it was necessary to change samples periodically. The intensities typically decayed by 0.3 to 0.6 dB during a run on a given sample.

Sample identity was confirmed by matching four of the lines to theoretical transitions (ref. 5) and by comparison with a previous recording of the spectrum made on the Hewlett-Packard 8400B spectrometer.

A sample pressure of 15 millitorr was registered as 39 millitorr by a thermocouple gage.

NAME: ETHANETHIOL					ID NO. 327.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26731.233	.02	64	51	5	2.6	-19	298	11
28088.212	.02	66	53	5	3.0	-18	297	11
28966.782	.02	65	51	5	2.1	-21	297	10
29126.752	.02	64	52	5	2.1	-18	297	12
29176.11	.10	65	51	2	3.0	-21	297	10
29603.035	.02	64	51	5	3.0	-18	298	11
29736.841	.02	63	49	5	2.1	-18	298	11
29745.096	.02	63	50	5	2.1	-18	298	11
30208.482	.02	65	51	5	2.1	-19	296	10
30322.85	.10	66	52	3	2.1	-20	297	10
30323.15	.10	66	52	2	2.6	-20	297	9
30394.008	.05	68	54	4	2.1	-19	297	10
30397.03	.10	61	45	4	2.6	-19	297	10
30397.26	.10	61	47	2	2.1	-19	297	10
30423.37	.10	64	48	4	2.1	-19	297	10
30448.52	.10	64	49	3	2.1	-19	297	10
30448.76	.10	64	50	2	1.7	-19	297	10
31092.323	.05	62	48	4	3.0	-18	297	10
31101.076	.02	63	49	4	2.1	-18	297	10
31307.509	.05	66	53	4	2.6	-19	297	10
31611.307	.05	68	54	4	2.6	-19	297	10
31845.996	.05	67	54	4	2.1	-19	297	10
32156.408	.02	64	50	5	3.0	-18	297	10
32170.246	.05	66	53	4	2.6	-18	297	10
32493.754	.02	64	51	5	2.1	-18	297	10
32501.167	.02	66	53	4	1.7	-18	297	10
32571.772	.02	63	50	4	2.1	-20	297	10
32802.707	.02	64	51	5	2.1	-19	297	10
32935.203	.02	64	51	4	3.4	-18	294	10
33352.515	.02	65	52	5	3.0	-18	297	10
33529.878	.05	66	53	4	2.6	-18	297	10
34407.168	.02	65	52	4	2.1	-17	297	10
34409.447	.02	66	53	5	2.6	-17	298	10
34444.456	.05	67	53	4	2.1	-17	296	10
34552.570	.05	68	55	4	2.6	-17	296	10
35155.886	.05	66	52	4	2.1	-17	296	10
35216.798	.02	63	50	4	2.1	-17	298	10
35338.151	.02	63	50	5	1.7	-17	298	10
35604.849	.02	63	50	5	2.6	-17	298	10
35784.983	.02	65	52	4	3.0	-17	298	10
35849.872	.02	66	53	4	2.1	-17	296	10
35916.399	.02	62	49	5	1.7	-17	298	10
36150.944	.02	64	51	4	2.6	-17	298	10
36151.92	.10	69	55	2	3.4	-17	298	10
36258.001	.02	63	50	5	3.0	-17	298	10
36749.794	.02	65	52	4	3.0	-17	298	10
36853.245	.02	64	50	5	2.1	-18	296	10
36907.472	.02	63	50	5	2.6	-16	296	10
37024.808	.02	66	53	5	2.6	-17	297	10
37454.511	.02	63	50	4	2.1	-17	297	10

NAME: ETHANETHIOL		CONTINUED				ID NO. 327.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
37965.175	.02	63	50	5	2.6	-17	297	10
38017.229	.02	65	52	5	3.0	-16	297	10
38274.840	.02	63	49	5	3.0	-17	297	10
38307.339	.05	64	51	4	2.1	-17	297	10
38323.109	.05	67	53	4	2.1	-17	297	10
38340.33	.10	65	53	3	1.7	-17	297	10
38395.973	.02	63	50	4	3.0	-17	297	10
38668.768	.02	62	49	5	3.0	-17	297	10
38757.394	.02	63	50	5	2.1	-17	297	11
39059.297	.02	63	49	4	2.1	-17	297	10
39652.332	.02	59	45	4	2.6	-16	297	10
39653.635	.02	59	45	4	2.6	-16	297	10
39958.148	.02	63	49	5	2.1	-19	297	10

## Ethylene glycol cyclic sulfite

Formula:  $\text{OCH}_2\text{CH}_2\text{OSO}$

CAS Registry number: 3741-38-6

Synonyms: ethylene sulfite, glycol sulfite

NBS identification number: 962.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich G720-8 with a stated purity of 97 percent. The sample partially decomposed on the initial chromatographic run with Chromosorb 102. This was a temperature-programed run to 200 °C. No problems were experienced at temperatures below 175 °C. A water peak of 0.07 percent was observed, as was one other impurity of 2.9 percent. This was distilled off at low temperature.

Remarks.- The sample adsorbed strongly and it was necessary to add sample periodically in order to maintain pressure. The lines are exceptionally broad and averaged more than 600 kHz at the 10 millitorr pressure used.

A sample pressure of 15 millitorr was registered as 45 millitorr on a thermocouple gage.

NAME: ETHYLENE GLYCOL CYCLIC SULFITE

ID NO. 962.00

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
32986.68	.20	65	46	3	3.4	-17	298	10
32994.132	.05	64	46	5	3.0	-17	298	10
35647.209	.05	63	45	4	2.1	-17	298	10
35717.09	.10	64		1	2.6	-16	298	10
36035.093	.05	65	47	4	3.8	-16	298	10
36603.570	.05	64	45	4	3.0	-16	298	10
36733.418	.02	65	46	5	2.1	-16	298	10
37946.33	.10	62	45	3	3.8	-17	297	10
37947.92	.20	65		1	3.8	-17	297	10
38059.990	.05	62	44	4	2.6	-17	296	10
38082.329	.05	63	45	4	3.4	-17	296	10
38196.615	.05	63	45	4	3.4	-17	296	10
38375.876	.05	62	44	5	3.8	-17	296	10
38500.139	.02	62	46	5	3.4	-16	297	10
38607.373	.05	62	44	4	3.8	-16	297	10
39504.725	.05	63	45	5	2.1	-16	297	10

## Formamide

Formula:  $\text{HCONH}_2$

CAS Registry number: 75-12-7

Synonym: methanamide

NBS identification number: 5.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Fisher F-82 Reagent grade. Chromatography on a Chromosorb 102 column showed impurities of about 0.04, 0.1, and 0.6 percent. Ammonia and methanol were identified in the first sample by their microwave spectra. The methanol was successfully distilled off, but the ammonia could not be entirely removed.

Remarks.- It was necessary to reduce sample pressure to 5 millitorr because of the broadness of the lines and the fine structure. Difficulty was experienced in maintaining a constant low pressure since the formamide was strongly adsorbed.

The concentration of ammonia was periodically checked and was never observed to exceed a few tenths of 1 percent.

The sample identity was verified by matching 21 of the lines with the theoretical spectrum given in reference 6.

NAME: FORMAMIDE							ID NO.	5.00
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
26758.21	.10	65	47	2	2.6	-19	297	5
26922.43	.10	65	47	3	1.7	-19	297	5
26923.08	.20	64	44	2	2.6	-19	298	4
27144.570	.02	65	47	5	2.1	-19	298	5
27397.64	.10	58	41	2	2.6	-19	298	5
27477.922	.01	65	49	5	2.1	-20	298	5
27514.210	.02	66	48	5	3.8	-20	298	5
27530.301	.02	64	45	4	2.6	-20	298	5
27752.55	.20	69	50	3	2.1	-19	298	5
28198.81	.10	63	45	2	2.1	-20	298	5
28335.60	.10	64	46	2	3.4	-18	298	5
28591.04	.10	64	46	3	3.8	-19	298	5
28591.76	.10	67	48	2	3.0	-19	298	5
28816.09	.10	57	39	2	2.1	-18	298	5
29745.355	.05	68	49	4	3.0	-18	298	5
30513.223	.05	61	43	4	2.6	-18	298	5
30736.426	.02	62	44	5	2.6	-18	298	5
31400.313	.02	63	44	4	2.6	-18	298	5
31692.715	.05	65	48	4	2.6	-18	298	5
31722.209	.02	66	49	4	2.6	-18	298	5
31724.13	.10	64	46	3	3.0	-19	298	5
31811.236	.05	68	49	4	2.6	-19	298	5
31825.294	.02	64	46	5	3.0	-19	298	5
32295.848	.02	59	42	4	2.1	-19	298	5
32297.88	.10	57	40	3	2.6	-19	298	5
32343.78	.10	68	50	3	2.1	-19	298	5
32515.614	.02	58	51	5	3.0	-19	298	5
33156.298	.05	71	52	4	2.1	-18	298	5
33306.42	.20	71	51	2	2.6	-18	298	5
33674.71	.10	69	51	2	3.0	-19	298	5
33987.67	.10	65	48	3	3.4	-18	298	5
33988.553	.02	63	45	4	3.0	-18	298	5
33991.08	.10	70	52	3	3.0	-18	298	5
34064.969	.02	68	50	5	3.8	-17	298	5
34182.56	.10	65	47	2	2.1	-19	298	5
34254.010	.05	63	44	4	2.6	-19	298	5
34663.23	.10	59	41	3	2.1	-19	298	5
34664.167	.02	56	38	4	3.4	-19	298	5
34993.95	.10	59	41	2	3.4	-18	298	5
35666.360	.02	67	49	4	3.4	-18	297	5
36162.005	.02	63	46	5	3.0	-17	297	5
36397.72	.10	62	44	2	3.8	-17	298	5
36608.85	.10	61	43	3	2.6	-18	298	5
37189.50	.10	55	37	2	3.8	-18	298	5
37259.594	.02	66	48	4	2.1	-18	298	5
37261.372	.02	63	46	4	3.8	-18	298	5
37406.494	.05	56	48	4	2.6	-18	298	5
37422.92	.10	68	50	2	2.1	-18	298	5
37566.91	.10	63	45	3	2.1	-18	298	5
37567.781	.02	60	42	4	2.6	-18	298	5

NAME: FORMAMIDE					CONTINUED				ID NO.	5.00
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr		
38365.24	.10	60	43	2	3.8	-18	298	5		
38827.517	.05	62	44	4	3.8	-17	298	5		
38828.40	.10	65	47	2	3.8	-17	298	5		
39460.636	.05	65	47	4	3.4	-17	298	5		
39563.123	.02	66	50	5	2.6	-17	298	5		
39742.25	.10	68	51	3	2.6	-17	298	5		
39743.057	.02	66	48	4	2.6	-17	298	5		



## Hydrocyanic acid

Formula: HCN

CAS Registry number: 74-90-8

Synonyms: hydrogen cyanide, prussic acid

NBS identification number: 4.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was prepared by the action of dilute hydrochloric acid on sodium cyanide in a flowing helium atmosphere, and the gas was trapped at liquid nitrogen temperature. Hydrochloric acid vapors were removed by vacuum distillation.

Remarks.- Since only two lines were observed, these were studied at several different pressures. The tabulated values are for 5 millitorr. Both lines show an apparent downward frequency shift of about 15 kHz at 10 millitorr and 20 kHz at 15 millitorr. The lines also show increases in peak intensity of about 10 and 20 percent at 10 and 15 millitorr, respectively.

These lines have both been verified theoretically (ref. 3).

A thermocouple gage read twice the true pressure at 10 millitorr and below, and read 26 millitorr at a true pressure of 15 millitorr.

NAME: HYDROCYANIC ACID						ID NO. 4.00		
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
29584.682	.02	57	41	4	3.4	-18	298	5
34953.794	.02	57	41	4	3.4	-18	298	5

## Isoxazole

Formula: N:CHCH:CHO

CAS Registry number: 288-14-2

NBS identification number: 333.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman 9530. Chromatography on a Chromosorb 102 column showed two impurities of about 0.1 percent each, one of 0.2 percent, and one of 0.4 percent.

Remarks.- Some of these lines are unusually broad and the shape suggests unresolved overlapping structure even though the lines are symmetrical. A few of the lines could not be completely modulated with a field of 3.8 kV/cm at a pressure of 10 millitorr.

NAME: ISOXAZOLE					ID NO. 333.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26544.043	.02	55.5	38.5		2.1	-18	298	10
26792.462	.01	51.8	34.8		3.0	-19	298	10
27061.074	.02	53.0	35.9		2.1	-19	298	10
27078.326	.01	55.7	39.0		2.1	-19	298	10
27216.323	.01	52.5	35.9		2.1	-18	298	10
27220.689	.02	53.3	36.1		2.1	-18	298	10
27459.260	.02	55.8	38.8		2.1	-19	298	10
27618.053	.02	54.5	37.5		3.0	-18	298	10
27634.448	.02	55.4	38.2		2.1	-18	298	10
27711.992	.02	51.9	35.0		3.8	-18	298	10
27812.491	.02	53.0	35.9		2.1	-18	298	10
27839.424	.01	52.5	35.7		2.1	-18	298	10
27900.093	.05	59	42	4	3.0	-18	296	10
28193.842	.02	55.1	37.6		1.7	-19	297	10
28624.168	.02	55.6	38.3		2.6	-18	297	10
28655.604	.02	51.4	34.2		3.4	-18	297	10
28675.989	.02	52.4	35.2		2.1	-18	297	10
28764.541	.01	52.3	35.6		2.1	-18	297	10
28881.931	.02	53.8	36.6		3.0	-17	294	10
28193.841	.02	55.2	37.6		1.7	-19	297	10
29210.012	.02	54.8	38.0		3.0	-17	297	10
29315.146	.02	55	38	4	3.0	-17	297	10
29575.874	.02	51.3	34.1		3.0	-18	297	10
29653.387	.02	52.2	35.1		2.1	-18	297	10
29738.589	.02	52.7	35.6		2.1	-18	298	10
29982.374	.01	53.0	35.9		3.0	-18	298	10
30006.247	.02	49.8	32.2		2.1	-20	298	10
30074.118	.02	55.5	38.2		3.8	-20	298	10
30208.454	.02	51.9	35.1		2.1	-19	298	10
30317.357	.01	51.5	35.1		3.0	-19	298	10
30346.913	.02	52	36	4	3.0	-19	298	10
30433.219	.02	51.2	34.1		3.0	-19	298	10
30533.965	.01	56.9	40.9		3.0	-18	298	10
30567.243	.02	55.0	37.7		3.0	-18	298	10
30631.297	.02	52.0	35.6		2.1	-18	298	10
30744.688	.02	52.0	34.8		2.1	-18	296	10
30903.356	.01	51.5	35.0		3.4	-17	296	10
30914.669	.02	53.3	36.3		3.4	-17	297	10
31046.834	.02	52.6	36.4		2.1	-18	297	10
31064.716	.02	55	37	4	2.1	-18	297	10
31198.537	.02	51.2	34.0		3.4	-18	297	10
31232.890	.01	54.1	37.4		2.6	-18	297	10
31681.813	.01	52.8	35.9		3.4	-18	297	10
31718.832	.01	51.1	34.6		3.4	-18	297	10
31839.795	.02	56	39	4	3.8	-17	298	10
31854.498	.01	51.2	34.2		3.0	-17	298	10
31948.061	.01	51.9	34.9		2.1	-17	298	10
32116.136	.01	52.5	36.4		2.1	-17	298	10
32294.273	.02	52.9	36.0		3.0	-17	298	10
32308.872	.01	52.5	35.4		2.1	-17	298	10

NAME: ISOXAZOLE		CONTINUED				ID NO. 333.00		
$\nu_0$ , MHz	$U$ , MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	$P$ , dBm	$T$ , K	$p$ , mtorr
32395.353	.01	51.2	34.3		3.0	-17	298	10
32711.749	.01	50.9	34.4		3.0	-17	298	10
32750.587	.02	51.3	35.2		1.7	-17	298	10
32768.464	.01	52.8	36.0		3.0	-17	298	10
32791.553	.02	52.0	35.7		2.1	-17	298	10
32825.126	.02	51.3	34.5		3.0	-17	298	10
32874.373	.02	54	37	4	2.1	-17	298	10
32910.184	.02	54.7	37.6		2.1	-17	298	10
33105.436	.02	56.0	40.0		1.7	-18	298	10
33119.524	.05	55	39	4	3.8	-18	298	10
33124.642	.02	53	36	4	2.6	-18	298	10
33154.828	.01	51.5	34.5		3.0	-18	298	10
33259.984	.02	51.8	34.7		2.1	-17	298	10
33384.196	.02	53	36	4	1.7	-18	298	10
33399.365	.01	51.6	34.3		3.8	-18	298	10
33408.288	.02	60	44	4	2.1	-18	298	10
33554.745	.01	52.6	36.8		1.7	-18	298	10
33562.167	.01	59	45	4	2.1	-18	298	10
33567.729	.02	53	36	4	3.4	-18	298	10
33574.864	.02	51.9	34.9		3.8	-18	298	10
33693.633	.02	52.4	36.7		3.8	-18	298	10
33696.691	.01	52.3	35.5		2.1	-18	298	10
33777.22	.20	54	38	3	1.7	-18	298	10
33778.34	.20	53	36	2	1.7	-18	298	10
33790.502	.02	49.0	31.7		1.7	-18	298	10
33803.104	.01	52.7	36.7		2.6	-18	298	10
33805.862	.02	53	37	4	3.4	-18	298	10
33809.72	.20	50	33	3	1.7	-19	296	10
33820.58	.20	52	35	3	2.6	-19	297	10
33821.55	.20	52	35	2	2.6	-19	297	10
33824.73	.20	52	35	3	3.8	-19	297	10
33825.64	.20	50	34	2	2.1	-19	297	10
33830.870	.05	52	35	4	3.4	-19	297	10
33841.64	.20	53	36	3	1.7	-19	297	10
33842.72	.20	53	36	2	1.7	-19	297	10
33857.373	.02	51	35	4	3.8	-19	297	10
33860.87	.20	50	33	2	3.0	-19	297	10
33863.461	.02	52	35	4	3.0	-19	297	10
33866.32	.20	53	36	3	1.7	-19	298	10
33867.887	.02	51	34	4	3.0	-19	298	10
33875.269	.01	52.2	35.9		1.7	-19	298	10
33882.482	.01	53.0	36.7		3.4	-19	298	10
33886.402	.02	53	37	4	3.8	-19	298	10
33892.82	.20	55	39	3	2.1	-19	298	10
33893.76	.20	55	38	2	2.1	-19	298	10
33943.45	.20	51	33	3	3.8	-19	298	10
33958.448	.01	52.6	35.5		3.4	-19	298	10
34078.467	.01	50.3	33.2		2.1	-19	298	10
34116.114	.01	52.7	35.7		3.0	-19	298	10
34195.774	.02	56	40	4	2.6	-18	298	10

NAME: ISOXAZOLE		CONTINUED				ID NO. 333.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
34273.453	.02	50.5	33.4		3.0	-18	298	10
34362.353	.02	52.4	35.3		3.0	-18	298	10
34539.339	.01	50.6	33.5		2.1	-18	298	10
34675.344	.02	51.7	34.6		2.1	-18	298	10
34724.323	.02	52.6	35.6		3.0	-18	298	10
34735.57	.10	54	37	6	2.15	-18	298	10
34846.694	.02	53.1	36.4		3.8	-17	298	10
34886.632	.02	50	33	4	2.1	-18	298	10
34894.360	.02	52.1	35.0		2.1	-18	298	10
35002.864	.02	51	34	4	3.8	-18	298	10
35209.310	.01	51.9	35.5		3.4	-18	298	10
35215.924	.02	54	37	4	3.8	-18	298	10
35233.282	.02	52.5	35.4		2.1	-18	298	10
35324.966	.02	50.4	33.2		2.1	-18	298	10
35351.432	.01	52.7	36.6		2.1	-18	297	10
35418.062	.01	51.4	34.6		3.0	-18	297	10
35445.835	.02	53.0	37.1		3.4	-18	297	10
35551.719	.02	53.5	37.7		2.1	-18	297	10
35578.479	.01	55.3	39.0		3.0	-18	297	10
35700.742	.01	52.5	36.6		2.1	-17	297	10
35862.946	.02	50.1	33.0		3.0	-17	297	10
35924.168	.02	52.6	35.6		2.1	-17	297	10
36043.360	.02	54	38	4	2.1	-18	298	10
36188.32	.20	49	32	2	3.0	-18	298	10
36281.444	.01	52.2	36.4		2.1	-18	298	10
36396.427	.05	52	35	4	3.0	-18	298	10
36402.089	.05	56	39	4	3.4	-18	298	10
36507.636	.02	50.2	33.0		2.1	-18	299	10
36640.26	.10	53	36	6	2.15	-17	299	10
36834.612	.02	53	36	4	2.1	-17	299	10
36935.433	.02	54.1	38.3		2.6	-16	299	10
37143.534	.01	51.8	35.8		3.0	-17	300	10
37264.466	.01	50.0	32.9		2.1	-18	300	10
37333.543	.01	49.8	32.8		3.0	-18	300	10
37465.289	.01	51.7	34.6		2.1	-17	300	10
37483.055	.02	50.6	34.1		3.0	-18	300	10
37757.924	.02	52.1	35.1		3.8	-18	300	10
37789.396	.01	51.3	34.3		2.1	-18	300	10
37839.563	.01	51.7	35.5		1.7	-18	300	10
37919.764	.01	54.4	38.1		3.0	-18	300	10
38003.506	.02	53.1	36.2		3.0	-17	300	10
38137.063	.02	50.0	33.1		3.0	-17	301	10
38162.724	.02	51.5	34.7		1.7	-18	300	10
38231.808	.02	54.0	38.2		2.1	-18	300	10
38234.242	.02	51.3	35.3		3.4	-18	300	10
38399.270	.01	49.6	32.7		3.0	-18	300	10
38580.95	.10	54	37	4	3.45	-18	300	10
38928.280	.02	51.8	35.0		3.0	-16	300	10
39127.125	.01	50.2	33.2		1.7	-16	299	10
39216.665	.02	56.4	39.0		2.1	-16	297	10

NAME: ISOXAZOLE		CONTINUED				ID NO. 333.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
39299.540	.01	57.5	41.5		1.7	-16	297	10
39358.015	.01	49.5	32.3		3.0	-16	297	10
39468.507	.02	53.0	35.7		2.1	-16	297	10
39472.235	.05	51	34	4	2.1	-16	297	10
39494.593	.01	51.1	34.8		3.0	-16	297	10
39713.83	.20	54	36	6	2.15	-16	298	10
39912.859	.05	51	34	4	2.1	-17	298	10
39914.684	.05	52	36	4	3.8	-17	298	10
39924.598	.02	54.8	39.0		1.7	-17	298	10
39998.68	.20	60	42	3	3.8	-16	298	10
40000.623	.02	51.6	34.6		3.0	-16	298	10

## Methanamine

Formula:  $\text{CH}_3\text{NH}_2$

CAS Registry number: 74-89-5

Synonyms: methylamine, aminomethane

NBS identification number: 125.00

Frequency range: 18 000 to 40 000 MHz

Sample.- The sample was Matheson bottled gas with a stated liquid-phase purity of 98 percent. This could not be verified by chromatography because the sample appeared to decompose partially in the chromatograph. Ammonia was detected in the sample cell at initial levels of less than 0.2 percent but increasing with time. The cell was evacuated and a fresh sample added before a concentration of 0.5 percent was reached.

Remarks.- Most of the lines exhibit some degree of asymmetry but the observed widths are not unusually large.

Sample identity was confirmed by theoretical verification of a number of lines in both the high and low frequency range (ref. 3).

Data below 26 500 MHz contain no information on Stark sensitivity or power level; however, the power levels were generally less than -15 dBm.



NAME: METHANAMINE						ID NO. 125.00		
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
18562.433	.02	69	58	5	2.1		300	11
18681.495	.02	67	54	5	2.1		300	11
19010.60	.20	70	57	3	3.0		301	13
19011.06	.10	68		1	2.6		301	13
19013.32	.10	53	41	3	2.1		300	11
19110.631	.05	59	46	4	1.7		300	12
19614.41	.10	69	57	4	2.1		301	13
19724.697	.10	59	47	3	2.1		300	12
19775.943	.05	69	57	4	2.1		300	12
19777.41	.10	67	55	3	3.4		300	11
19919.44	.10	57	45	3	2.6		300	11
19933.611	.05	66	53	4	2.6		299	11
20075.99	.10	53	41	3	2.1		299	11
20243.465	.05	58	45	4	2.1		299	11
20302.765	.02	69	58	5	2.6		299	11
20325.75	.10	68	57	2	2.1		299	11
20547.290	.02	60	48	4	2.1		298	11
20831.181	.02	60	47	4	2.1		298	11
20911.589	.05	70	58	5	1.7		298	11
20947.195	.02	69	58	5	2.1		298	11
20971.91	.10	66	54	2	3.0		298	11
20973.213	.05	65	53	5	2.1		299	11
20994.627	.02	64	53	5	2.1		299	11
21012.861	.05	66	53	4	2.6		299	11
21019.074	.05	60	48	4	2.1		299	11
21026.51	.10	66	54	3	2.1		299	11
21035.23	.10	67	54	3	1.7		299	11
21051.541	.05	60	48	7	1.7		299	11
21202.703	.02	70	58	4	3.0		299	11
21296.893	.05	58	45	4	2.1		299	11
21478.84	.10	66	54	2	1.7		299	11
21615.130	.02	64	53	4	2.1		299	12
21682.14	.10	70	58	2	1.7		299	12
21705.67	.10	69	58	3	3.4		299	12
21712.642	.02	60	48	7	3.0		299	12
21765.13	.10	57	45	3	2.1		299	12
21841.833	.05	51	39	3	2.1		299	12
21930.00	.10	65	51	4	1.7		299	12
21931.421	.05	67	55	5	1.7		299	12
22060.433	.02	64	53	5	2.1		299	12
22080.771	.02	69	58	5	2.6		299	12
22112.106	.05	64	51	5	2.6		299	12
22221.214	.02	68	57	5	3.0		299	12
22258.386	.05	57	44	4	2.1		299	12
22369.40	.10	71	59	3	2.6		299	12
22369.807	.05	69	56	4	2.6		299	12
22381.975	.05	69	56	4	1.7		299	12
22527.95	.10	51	39	3	2.1		298	12
22581.447	.02	64	52	4	3.0		298	12
22588.287	.02	65	53	4	2.1		298	12

NAME: METHANAMINE		CONTINUED				ID NO. 125.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
22722.579	.02	59	47	7	2.6		298	12
22759.22	.10	55	43	3	2.1		298	12
22765.701	.05	69	58	5	1.7		299	12
22818.675	.05	69	58	5	1.7		299	12
22980.893	.02	60	48	7	2.6		299	12
22981.54	.10	63	52	2	2.1		299	12
23071.187	.02	66	54	4	2.1		299	12
23071.76	.10	69	57	2	2.1		299	12
23091.15	.10	69	58	3	2.6		299	12
23091.64	.10	69	58	2	3.0		299	12
23118.964	.05	57	44	4	2.1		299	11
23219.156	.05	63	50	5	3.4		299	11
23300.84	.10	66	53	2	2.1		299	11
23311.30	.10	65	53	2	1.7		299	12
23315.551	.02	64	52	4	2.1		300	12
23340.726	.02	62	49	4	2.1		300	12
23341.32	.10	64	52	2	1.7		300	12
23409.218	.05	60	48	7	2.1		300	12
23429.369	.05	60	48	7	2.1		300	12
23432.830	.02	64	53	4	2.1		300	12
23449.43	.10	63	51	3	2.1		300	12
23450.153	.02	61	48	5	2.1		300	12
23526.994	.02	71	60	4	2.1		301	12
23608.24	.10	71	59	3	1.7		301	12
23683.316	.02	59	46	4	2.6		301	12
23861.302	.02	59	47	4	2.6		301	12
23873.497	.05	56	44	4	3.0		302	12
24019.04	.10	57	45	3	2.1		302	12
24037.161	.02	72	61	4	2.1		302	12
24078.794	.05	67	56	5	2.6		302	12
24889.386	.05	50	38	3	2.1		299	12
24889.77	.10	52	40	2	2.6		299	12
24993.724	.02	65	51	5	1.7		299	12
25015.92	.10	66	54	2	2.1		299	12
25063.513	.02	56	45	7	3.0		299	12
25176.521	.02	71	59	4	2.1		300	12
25206.60	.10	50	38	3	2.1		300	12
25401.540	.05	62	49	5	2.1		300	12
25473.44	.10	67	55	3	2.1		300	12
25507.462	.02	56	45	7	3.0		300	12
25633.930	.02	69	57	5	2.1		300	12
25665.13	.10	70	57	2	1.7		300	12
25725.940	.02	66	55	5	3.0		301	12
25737.634	.02	69	57	4	2.6		301	12
25810.46	.10	55	43	3	3.0		301	12
26134.670	.02	57	45	4	2.1		301	12
26165.90	.10	70	59	3	1.7		301	12
26205.709	.02	69	57	4	2.1		301	12
26339.451	.02	57	46	4	2.1		301	12
26447.854	.05	61	49	5	2.1		301	12

NAME: METHANAMINE			CONTINUED			ID NO. 125.00		
$\nu_0$ , MHz	$U$ , MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	$P$ , dBm	$T$ , K	$p$ , mtorr
26487.025	.05	57	45	7	1.7		301	12
26493.502	.05	56	44	3	2.6		301	12
26588.699	.01	56	44	4	2.1	-15	301	10
26655.004	.05	57.3	44.8		2.15	-19	300	10
26695.331	.05	59	46	4	2.15	-19	300	10
26717.79	.20	61	48	2	1.75	-19	300	9
26728.85	.50	64	48	2	1.75	-19	300	10
27445.26	.10	60	46	6	2.15	-18	300	10
27504.936	.01	62	50	5	1.7	-19	300	10
27758.477	.01	62	50	5	2.1	-18	300	10
28107.729	.05	48	36	3	2.1	-18	300	10
28108.099	.05	50	38	2	2.1	-18	300	10
28143.078	.01	48	36	4	2.1	-18	300	10
28143.531	.05	50	38	2	3.0	-18	300	10
28380.88	.10	59	46	6	2.15	-18	300	10
28418.042	.01	65	53	4	2.1	-17	300	10
28513.352	.02	56	43	4	2.1	-18	300	10
28651.095	.01	58	46	4	2.1	-18	299	10
28651.779	.02	60	48	4	2.6	-18	299	10
28909.51	.10	63	51	3	2.1	-18	299	10
28909.99	.10	63	50	2	2.1	-18	299	10
28931.25	.10	64	52	2	3.4	-18	299	10
29055.141	.02	53	40	4	2.1	-17	299	10
29055.615	.05	55	42	2	3.0	-17	299	10
29098.557	.01	61	50	5	2.1	-17	299	10
29138.56	.10	64	51	4	1.75	-18	299	10
29147.358	.01	64	51	5	1.7	-18	299	10
29163.555	.01	64	52	5	1.7	-17	299	11
29191.791	.05	53	41	3	2.1	-17	299	10
29243.81	.10	59	46	4	1.75	-17	299	10
29306.697	.02	66	53	4	2.1	-17	299	10
29307.425	.02	63	50	4	2.6	-17	299	10
29599.534	.01	64	52	4	2.1	-18	300	10
29636.95	.20	66	52	4	2.15	-18	300	10
30025.686	.05	58	45	4	2.15	-18	300	10
30088.290	.01	59.9	48.0		2.1	-18	299	10
30226.40	.10	62	49	3	2.1	-18	296	9
30236.450	.01	59.7	47.7		2.6	-18	296	10
30566.14	.10	55	52	3	3.0	-17	296	10
30721.043	.01	57.6	44.8		2.1	-17	296	10
30828.990	.01	63	50	4	2.1	-18	296	10
30974.362	.05	63	50	4	2.1	-19	297	10
30993.838	.01	63	51	5	3.0	-19	297	10
30997.136	.01	63	51	5	3.0	-19	297	10
31054.69	.10	64	52	3	2.1	-19	297	11
31140.273	.02	62	47	4	3.0	-19	297	10
31220.591	.02	47	34	4	2.1	-18	297	10
31221.016	.05	49	37	2	2.6	-18	297	10
31327.539	.05	57.7	44.8		2.15	-19	297	10
31583.111	.01	46	34	4	2.1	-19	297	10

NAME: METHANAMINE		CONTINUED				ID NO. 125.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
31583.617	.05	49	36	2	2.1	-19	297	10
31845.857	.01	57.3	44.7		2.1	-19	298	10
32103.680	.01	62	49	4	2.1	-19	298	10
32112.273	.05	52	40	3	2.1	-19	298	10
32112.63	.10	54	42	2	2.1	-19	298	10
32154.923	.01	61	49	5	3.0	-18	298	10
32186.665	.01	61	49	5	2.1	-19	298	10
32279.388	.01	57.2	44.8		1.7	-18	298	10
32282.12	.10	62	49	3	1.7	-19	298	10
32282.842	.01	59.5	45.9		1.7	-19	298	10
32287.224	.01	60	48	4	2.1	-19	298	10
32306.035	.02	60	47	4	1.7	-19	298	10
32467.649	.01	51.3	38.6		2.6	-19	298	10
32468.181	.05	54	41	2	2.6	-19	298	10
32469.11	.10	60	47	2	3.0	-19	298	10
32633.820	.01	57.2	44.9		3.0	-19	298	10
32708.44	.10	61	49	3	2.1	-19	298	10
32916.550	.01	57.3	45.2		3.4	-19	298	10
33136.116	.01	57.6	45.6		2.1	-18	298	10
33152.026	.01	55.7	43.5		2.6	-18	298	10
33301.610	.01	57.8	45.8		3.0	-17	298	10
33388.189	.05	63	50	4	2.1	-18	298	10
33419.914	.02	61	48	4	3.0	-18	298	10
33422.188	.01	58.5	46.4		2.1	-18	298	10
33506.547	.01	59.2	46.9		1.7	-19	298	10
33563.115	.01	60.2	47.5		2.1	-19	298	10
33598.815	.02	62	48	4	2.1	-19	298	10
33619.90	.10	64	51	2	1.75	-19	298	10
33862.114	.01	63	51	5	1.7	-18	298	9
33989.055	.01	64	52	5	2.1	-18	298	9
34313.653	.01	55.1	43.0		2.1	-18	298	10
34314.367	.02	58	45	4	2.6	-18	298	10
34527.388	.02	45	32	4	2.1	-18	298	10
34527.869	.05	48	35	2	2.6	-18	298	10
34623.524	.01	60.1	47.6		1.7	-18	298	10
34772.896	.02	59	46	4	2.1	-18	298	10
34834.383	.01	61	49	5	1.7	-18	298	10
34835.030	.02	64	51	4	1.7	-18	298	10
34896.55	.10	65	52	3	1.75	-18	298	10
34907.50	.10	61	49	3	2.6	-18	298	10
35182.679	.01	45	32	4	2.1	-15	296	10
35183.242	.05	47	35	2	2.1	-15	296	10
35247.593	.05	50	38	3	2.1	-15	296	10
35247.996	.05	52	40	2	2.1	-15	296	10
35429.905	.02	63	50	4	2.1	-15	296	10
35584.904	.01	64	51	5	2.1	-15	296	10
36014.855	.01	50	37	4	2.6	-18	297	10
36015.440	.05	52	39	2	3.4	-18	297	10
36034.872	.01	62	49	5	3.8	-18	297	10
36066.787	.02	55	42	4	1.7	-17	297	10

NAME: METHANAMINE			CONTINUED			ID NO. 125.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
36156.630	.02	59	46	4	2.1	-16	297	10
36226.769	.01	64	52	4	2.1	-16	297	10
36231.547	.01	64	51	4	1.7	-16	297	10
36399.981	.01	61	50	5	2.1	-16	297	10
36451.310	.01	60.2	48.1		2.1	-16	297	10
36452.81	.10	59	46	3	3.4	-16	297	10
36792.561	.01	55.6	42.8		3.0	-16	297	10
36885.13	.10	60	48	3	2.1	-16	297	10
36957.60	.10	60	47	3	2.1	-17	297	10
37233.59	.10	60	47	3	2.1S	-16	297	10
37563.707	.02	58	45	4	2.1	-16	297	10
37854.714	.01	60	48	4	1.7	-16	297	10
37938.678	.01	65	53	5	2.1	-16	297	10
37956.96	.10	64	51	3	2.6	-16	297	10
38002.963	.01	44	32	4	2.1	-18	297	11
38003.501	.05	47	34	2	2.6	-18	297	10
38123.912	.02	64	51	4	1.7	-18	297	10
38166.599	.02	59	46	4	2.1	-18	297	10
38193.123	.01	59.6	47.9		3.4	-18	297	10
38216.591	.02	59	45	4	2.1	-18	297	10
38252.245	.05	53	41	3	2.1	-18	297	10
38583.978	.01	49	37	4	2.1	-18	297	10
38584.439	.05	52	40	2	2.1	-18	297	10
38840.86	.10	61	47	2	2.6	-15	297	10
38859.788	.05	58.7	46.2		2.6S	-16	298	10
38908.278	.01	44	32	4	2.1	-16	298	10
38908.896	.05	47	34	2	2.1	-16	298	10
38910.34	.10	64	49	2	2.1	-16	298	10
38921.48	.10	59	46	3	3.0	-16	298	10
38985.180	.02	56	43	4	2.1	-15	295	10
39127.449	.05	59	47	3	2.1	-16	296	10
39363.352	.01	61	49	4	2.1	-14	296	10
39444.262	.01	65	53	5	2.1	-14	296	10
39518.276	.05	54.7	42.6		1.7S	-15	294	10
39521.529	.05	55	43	4	2.1S	-15	294	10
39656.502	.01	48.5	36.0		3.0	-14	295	10
39657.143	.05	51	39	2	3.4	-14	295	10
39776.931	.01	63	51	4	2.1	-15	295	10
39868.770	.05	61	49	3	2.1	-13	295	10
39869.37	.10	59	47	3	2.6	-13	295	10
39928.451	.01	53.5	41.2		2.1	-15	295	10
39929.192	.02	56	44	4	2.6	-15	295	10
39948.309	.05	54	41	2	1.7	-15	295	10

## Methanethiol

Formula:  $\text{CH}_3\text{SH}$

CAS Registry number: 74-93-1

Synonym: methyl mercaptan

NBS identification number: 47.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Matheson bottled gas with a stated purity of 99.5 percent or better. Chromatography on a Chromosorb 102 column showed one impurity peak of 0.1 percent.

Remarks.- This sample initially reacted in the cell to form sulfur dioxide, and a stable pressure could not be maintained. However, after a conditioning period the effect was greatly reduced and it became possible to obtain the spectrum. It was necessary to change the sample periodically to keep the observed intensities from decaying by more than 0.4 dB during a run. The intensity decay rate was measured for each sample and the tabulated intensities were corrected. Spot checks showed agreement generally to within 0.1 dB between corrected intensities and those remeasured with a fresh sample.

The spectrum of methanethiol has been theoretically verified and a list of numerous lines has been published (ref. 3).

NAME: METHANETHIOL

ID NO. 47.00

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
26994.09	.10	64	52	4	2.15	-20	298	15
27333.950	.02	61	49	5	2.6	-18	298	15
27364.334	.02	63	50	5	2.1	-20	298	15
27911.910	.05	66	53	5	2.1	-18	299	15
28911.020	.02	65	53	4	3.0	-18	299	14
28990.253	.02	65	53	5	2.1	-18	299	15
29074.186	.05	66	55	5	2.6	-17	299	15
29091.821	.02	62	49	5	2.1	-18	299	15
29593.437	.02	62	49	4	2.1	-18	299	15
30083.356	.02	65	53	5	2.1	-18	299	15
30367.844	.05	64	52	4	2.1	-18	299	15
30508.784	.02	59.9	47.5		3.4	-18	297	15
30626.468	.02	63	51	5	2.1	-18	297	14
30652.227	.02	63	51	5	1.7	-18	297	15
30741.777	.02	58.7	46.2		2.1	-18	297	15
30859.739	.02	63	51	5	2.1	-18	297	15
30874.767	.02	59.7	47.2		2.1	-18	297	15
30972.784	.02	61	48	5	2.1	-17	297	15
31068.296	.02	62	50	4	2.1	-18	298	15
31252.997	.02	62	49	5	2.1	-17	298	15
31414.869	.02	62	49	5	2.1	-19	298	15
31555.112	.02	61	49	5	2.1	-18	298	15
31675.040	.02	61	48	4	2.1	-18	298	15
31776.034	.02	60	48	4	2.1	-18	298	15
31859.628	.02	60.1	47.4		3.0	-17	298	15
31927.291	.02	60	47	4	2.1	-17	298	17
31980.641	.02	59.6	47.0		1.7	-18	297	15
31994.808	.05	66	54	5	2.15	-17	298	15
32002.285	.05	65	53	5	2.15	-17	298	15
32011.735	.05	63	51	5	2.15	-17	298	16
32021.196	.02	59.5	46.9		1.7	-17	298	16
32022.754	.02	61	48	5	3.4	-17	298	15
32034.81	.10	60	48	6	2.15	-19	297	15
32047.25	.10	60	47	6	2.15	-19	297	15
32050.50	.10	59	46	4	2.15	-19	297	15
32059.36	.10	60	47	6	2.15	-19	298	15
32070.16	.10	56	43	6	2.15	-19	297	15
32078.99	.10	59	46	6	2.15	-19	298	15
32081.34	.10	59	46	6	2.15	-19	298	15
32084.54	.10	59	46	4	2.15	-17	299	15
32085.71	.10	59	46	4	2.15	-17	299	15
32820.753	.05	65	52	5	1.75	-17	299	15
32827.938	.05	63	51	5	2.15	-17	299	15
32844.359	.05	62	50	5	2.15	-17	299	15
32874.205	.05	62	49	5	2.15	-18	299	15
32880.07	.10	60	48	6	2.15	-17	298	15
32922.320	.05	51	48	5	2.15	-18	299	15
32994.119	.05	61	48	5	2.15	-18	299	15
33077.843	.02	59.3	47.0		1.7	-18	299	15
33095.66	.10	60	47	4	2.15	-18	299	15

NAME: METHANETHIOL			CONTINUED			ID NO. 47.00		
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
33096.681	.02	59	46	4	3.8	-18	298	15
33233.53	.10	60	47	4	2.1S	-18	298	15
33414.85	.10	60	47	6	2.1S	-18	298	15
33647.26	.10	60	47	4	2.1S	-19	299	15
33658.679	.02	63	52	5	2.1	-19	299	15
33828.985	.02	63	51	5	2.1	-19	297	16
33858.769	.02	64	52	5	1.7	-18	297	15
33938.79	.10	60	46	6	2.1S	-18	298	15
34193.084	.02	58.5	46.0		3.0	-17	298	15
34298.02	.10	59	47	6	2.1S	-17	297	15
34488.167	.05	64	52	5	2.1S	-17	298	16
34527.332	.02	58.6	45.9		2.1	-17	298	15
34733.88	.10	59	46	6	2.1S	-17	298	15
34942.791	.05	66	54	4	2.1S	-17	298	15
35093.950	.02	63	50	5	2.1	-17	298	15
35167.526	.02	63	51	5	1.7	-18	298	15
35254.573	.02	60	47	4	2.1	-18	298	15
35255.76	.10	60	46	4	3.0S	-18	298	15
35543.24	.10	59	47	4	2.1S	-18	298	15
35547.150	.05	65	54	5	2.1S	-18	299	15
35857.420	.05	61	49	5	2.1S	-17	299	15
35873.43	.10	59	47	4	2.1S	-17	298	15
35913.530	.02	62	49	5	2.1	-17	299	15
36597.11	.10	59	46	6	2.1S	-17	298	15
37293.326	.01	57.2	45.0		3.8	-18	298	15
37409.943	.02	64	52	5	2.1	-17	299	15
37437.43	.10	59	46	6	2.1S	-17	298	15
38054.483	.02	64	52	4	2.6	-17	299	15
38225.355	.02	63	51	5	3.4	-18	299	15
38405.45	.10	59	46	6	2.1S	-17	298	15
38650.986	.02	63	50	5	1.7	-17	297	15
38981.630	.02	61	49	5	2.1	-17	297	15
39512.66	.10	59	46	6	2.1S	-16	297	15
39877.333	.05	62	50	4	2.1S	-18	296	15



## Methyl sulfide

Formula:  $\text{CH}_3\text{SCH}_3$

CAS Registry number: 75-18-3

Synonyms: dimethyl sulfide, methylthiomethane

NBS identification number: 326.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman 1106. Chromatography on a Chromosorb 102 column showed two impurities of less than 0.1 percent each.

Remarks.- The spectrum contains a number of triplets with a spacing of about 0.5 MHz. The separation was sufficient for good frequency measurements, but the line widths of the center components could not be measured in most cases.

The sample identity has been verified by matching a number of lines with their published theoretical assignments (ref. 3).

The 12-millitorr sample pressure was registered as 37 millitorr on a thermocouple gage.

NAME: METHYL SULFIDE							ID NO. 326.00	
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
27787.12	.10	61	48	3	3.0	-18	297	12
27787.634	.05	59		1	2.1	-18	297	12
27788.16	.10	61	48	2	3.0	-18	297	12
27832.12	.10	64	51	3	2.1	-18	297	12
27832.651	.02	60	47	4	2.1	-18	297	12
27833.18	.10	63	50	2	2.1	-18	297	12
27850.799	.02	65	53	5	1.7	-18	297	12
27864.772	.02	63	51	4	2.1	-18	297	12
27877.86	.10	67	54	2	2.1	-18	297	12
27890.772	.02	64	51	5	2.6	-18	297	12
27947.853	.02	65	52	5	1.7	-18	297	12
28011.232	.02	67	54	5	3.0	-18	297	12
28021.630	.05	68	55	4	3.0	-18	298	12
28025.461	.02	65	52	5	3.0	-18	298	12
28226.954	.05	68	56	4	3.0	-18	298	12
28343.904	.05	67	55	4	1.7	-17	298	12
28346.992	.02	65	53	4	3.0	-17	298	12
28350.069	.05	68	55	4	3.0	-18	298	12
28385.68	.10	70	56	2	2.1	-17	298	12
28423.345	.05	69	57	4	1.7	-17	298	12
28425.319	.02	66	54	5	2.1	-17	298	12
28449.751	.05	67	55	4	2.6	-17	298	12
28456.365	.05	69	56	5	3.4	-17	298	12
28542.364	.05	68	56	4	1.7	-17	298	12
28681.312	.05	68	56	4	2.1	-18	298	12
28738.693	.05	68	55	4	3.8	-18	298	12
29060.29	.10	64	51	3	3.0	-19	297	12
29060.869	.02	62	48	5	2.1	-20	297	12
29061.45	.10	64	51	2	2.1	-19	297	12
29194.041	.02	66	54	4	1.7	-19	297	12
29286.543	.02	66	54	5	2.1	-19	297	12
29363.17	.10	68	55	4	2.15	-20	297	12
29387.829	.02	64	52	4	3.0	-19	297	12
29400.129	.02	62	50	4	2.1	-19	297	12
29410.667	.02	66	54	4	3.4	-20	297	12
29412.23	.10	66	54	3	3.4	-20	298	12
29452.92	.10	61	48	3	2.1	-20	298	12
29453.402	.01	58.1	44.6		2.1	-19	298	12
29453.89	.10	61	48	2	1.7	-19	298	12
29455.00	.10	66	53	2	2.1	-20	298	12
29468.486	.02	62	50	5	2.6	-20	298	12
29720.113	.05	68	56	5	2.1	-20	298	12
29773.426	.05	68	55	5	1.75	-20	298	12
29844.842	.05	68	56	4	2.1	-20	298	12
29938.183	.05	68	55	4	1.7	-20	298	12
29940.551	.05	68	56	4	2.6	-19	298	12
29943.843	.05	64	52	5	2.15	-19	298	12
29947.150	.05	69	56	4	2.6	-19	298	12
29995.878	.05	69	56	5	1.7	-20	298	12
30001.276	.05	69	56	4	2.1	-19	298	12

NAME: METHYL SULFIDE			CONTINUED			ID NO. 326.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
30003.03	.10	69	56	2	3.0	-19	298	12
30080.438	.05	68	56	5	2.6	-20	298	12
30322.628	.05	67	55	5	2.6	-19	298	12
30363.820	.02	67	55	5	2.6	-19	297	12
30372.280	.05	69	57	4	3.0	-19	297	12
30383.270	.02	65	53	5	2.1	-18	297	12
30399.884	.05	68	56	4	2.6	-18	297	12
30414.421	.05	68	55	5	2.1	-18	297	12
30464.885	.05	70	57	4	1.7	-18	297	12
30542.611	.02	61	49	4	3.8	-18	297	12
30676.521	.05	66	54	4	3.0	-18	297	12
30688.420	.02	64	52	5	2.6	-18	297	12
30700.215	.05	67	54	4	1.7	-18	297	12
30806.946	.05	58		1	2.6	-18	298	12
30807.36	.10	65	52	2	2.15	-18	298	12
30822.86	.10	62	49	3	3.8	-18	298	12
30823.322	.05	60		1	3.8	-17	298	12
30823.7P	.10	62	49	2	3.8	-18	298	12
30954.984	.05	69	57	4	2.6	-18	298	12
31036.699	.05	69	56	4	2.6	-17	298	12
31093.936	.05	68	56	5	2.6	-17	298	12
31097.661	.05	66	54	4	2.6	-17	298	12
31280.327	.05	68	56	4	2.6	-18	298	12
31371.250	.05	68	56	4	1.7	-18	298	12
31372.992	.02	65	52	5	3.4	-18	298	12
31618.234	.05	67	55	5	1.75	-17	298	12
32763.518	.05	67	54	4	3.0	-18	298	12
32770.358	.02	65	52	4	3.0	-17	297	12
32777.063	.05	67	55	4	3.4	-18	297	12
32918.193	.02	65	53	5	2.1	-18	297	12
32930.734	.02	61	48	5	3.0	-18	297	12
32943.42	.10	66	53	2	3.4	-18	297	12
32968.649	.05	68	54	4	1.7	-18	297	12
32969.61	.10	68	54	3	2.1	-18	297	12
32970.23	.20	68	53	2	2.1	-18	297	12
33125.650	.02	63	50	5	2.1	-18	297	12
33139.378	.02	61	48	5	3.4	-18	297	12
33152.936	.05	64	50	4	1.7	-18	298	12
33210.68	.10	58	45	3	2.1	-18	298	12
33211.204	.05	56		1	2.1	-18	298	12
33211.72	.10	58	45	2	2.6	-18	298	12
33260.396	.05	68	55	4	1.7	-18	298	12
33300.140	.02	66	54	5	1.7	-18	298	12
33498.679	.05	67	54	4	2.6	-18	298	12
33622.890	.02	65	52	4	2.6	-19	298	12
33626.638	.02	63	50	5	2.1	-19	298	12
33630.375	.02	65	53	4	2.6	-19	298	12
33744.517	.02	64	52	4	2.1	-18	298	12
33790.937	.05	68	55	5	2.6	-18	298	12
33961.84	.10	69	56	3	1.7	-18	298	12

NAME: METHYL SULFIDE			CONTINUED			ID NO. 326.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
33969.651	.05	66	54	4	2.1	-18	298	12
34139.612	.05	69	57	5	2.1	-18	298	12
34205.046	.05	69	55	4	1.7	-17	298	12
34212.61	.10	69	57	2	2.6	-17	298	12
34573.024	.05	70	57	4	1.7	-17	298	12
34631.401	.05	69	56	4	3.0	-17	298	12
34653.212	.02	67	54	5	2.1	-17	298	12
34804.20	.10	68	55	3	3.4	-17	298	12
34804.601	.05	68		1	2.1	-17	298	12
34805.34	.10	68		1	2.6	-17	298	12
34820.039	.05	68	55	5	1.7	-17	298	12
34920.141	.05	68	56	5	2.1	-17	298	12
34925.790	.02	66	54	5	2.1	-17	298	12
34963.056	.02	60.2	45.5		2.6	-17	296	12
34969.73	.10	69	57	3	3.0	-17	296	12
34970.516	.05	65	53	4	2.6	-17	297	12
35135.229	.05	68	55	4	2.6	-17	297	12
35214.547	.05	64	49	4	3.0	-17	297	12
35364.496	.05	66	53	4	2.6	-17	297	12
36273.78	.10	66	53	3	1.7	-17	297	12
36274.520	.02	64	51	5	2.1	-17	297	12
36275.25	.10	66	53	2	2.6	-17	297	12
36619.876	.05	66	53	5	1.7	-16	297	12
36621.37	.10	65	51	3	2.1	-16	297	12
36623.049	.05	68	52	4	2.1	-16	297	12
36909.83	.10	68	54	3	1.7	-16	297	12
36910.554	.05	68		1	1.7	-16	297	12
37116.315	.05	67	53	4	1.7	-17	297	12
37117.311	.02	65	51	5	2.1	-17	297	12
37192.764	.05	67	54	5	1.75	-17	297	12
37534.172	.05	65	52	4	2.6	-17	297	12
37847.682	.05	67	55	4	2.6	-18	297	12
38262.593	.05	67	53	4	2.6	-17	297	12
38263.34	.20	66	53	3	1.75	-17	297	12
38264.015	.05	65	51	4	2.1	-17	297	12
38264.75	.10	68	54	2	1.7	-17	297	12
38333.843	.05	68	55	4	2.1	-17	297	12
38341.030	.02	63	51	4	2.6	-17	298	12
38348.055	.05	68	55	5	3.4	-17	298	12
38475.075	.05	67	54	5	2.15	-17	298	12
38701.088	.02	61	49	5	2.1	-17	298	12
38714.831	.02	59.8	47.0		2.1	-17	298	12
38728.663	.02	62	49	5	1.7	-17	298	12
38832.981	.05	67	55	4	1.7	-17	298	12
38983.009	.05	66	44	4	2.15	-17	298	12
39016.342	.02	66	53	5	2.6	-15	296	12
39091.833	.02	64	51	5	3.4	-15	296	12
39106.570	.02	60	47	4	3.0	-16	296	12
39121.221	.02	64	51	5	1.7	-16	297	12
39272.12	.10	65	52	3	2.6	-16	297	12

NAME: METHYL SULFIDE

CONTINUED

ID NO. 326.00

$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
39272.867	.02	61	48	5	2.1	-16	297	12
39273.52	.10	65	52	2	1.7	-16	297	12
39285.68	.10	59	46	3	2.1	-16	297	12
39286.230	.01	55.6	42.4		2.1	-16	297	12
39286.78	.10	59	46	2	2.1	-16	297	12
39305.13	.10	68	56	4	2.15	-15	297	12
39308.242	.02	65	53	5	2.1	-15	297	12
39309.776	.05	68	56	5	2.6	-15	297	12
39338.90	.10	65	53	3	2.6	-16	297	12
39349.893	.02	67	54	5	2.6	-16	297	12
39355.25	.10	65	53	3	2.6	-16	297	12
39418.004	.02	65	53	5	2.1	-16	297	12
39431.817	.02	63	50	5	3.0	-16	297	12
39445.670	.05	66	52	4	3.0	-16	297	12
39576.54	.10	69	56	5	2.15	-15	297	12
39625.912	.02	66	53	5	2.1	-15	298	12
39630.398	.02	61	49	5	3.4	-15	298	12
39634.896	.02	66	53	5	3.4	-15	298	12
39668.975	.05	69	57	4	2.6	-16	298	12
39805.833	.02	64	51	5	3.0	-17	298	12
39852.965	.05	67	54	4	2.15	-16	298	12
39867.936	.02	62	50	5	2.1	-17	298	12
39882.918	.05	67	53	4	3.0	-17	298	12

## Methyl thiirane

Formula:  $\text{SCH}_2\text{CHCH}_3$

CAS Registry number: 1072-43-1

Synonym: propylene sulfide

NBS identification number: 194.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich P5,320-9 with a stated purity of 98 percent. Sample identity was confirmed by the manufacturer by gas chromatography and infrared analysis. Chromatography on a Chromosorb 102 column showed six impurities. Three were 0.01 percent or less, and the concentrations of the others were 0.04, 0.13, and 0.44 percent.

Remarks.- The sample was held at low temperature in the manifold to pump off any impurities which were more volatile than the methyl thiirane. After this procedure, no difference was noted between measurements made on a sample distilled into the cell at low temperature and measurements made on samples taken at room temperature.

Measurements were initially made at a pressure of 15 millitorr, but the line widths were in the vicinity of 0.5 MHz; therefore, the measurements were repeated at lower pressure.

NAME: METHYL THIIRANE							ID NO. 194.00	
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	n, mtorr
27414.398	.01	59.8	45.2	4 4	2.1	-17	297	10
27657.843	.02	59	44		3.0	-17	297	10
28468.763	.02	60	46		3.0	-16	297	10
29039.058	.01	58.4	43.9		2.1	-16	298	10
31678.921	.01	57.3	42.9		2.1	-16	298	10
33248.992	.01	58.6	43.7		2.1	-17	298	10
33692.594	.01	59.0	44.6		3.0	-18	298	10
34417.493	.01	58.1	43.2		3.0	-18	298	10
35175.539	.01	59.2	44.2		2.1	-18	298	10
35608.009	.01	56.5	41.9		2.1	-16	298	10
36141.938	.01	55.9	41.2		2.1	-14	297	10
36701.421	.01	56.0	41.4		2.1	-15	298	10
36805.675	.01	55.5	40.8		3.8	-15	297	10
36887.926	.01	57.8	42.6		3.0	-16	296	10
38229.833	.01	56.0	41.4		2.1	-16	298	10
38853.372	.01	55.0	40.3		2.1	-15	297	10
39697.758	.01	57.2	42.7		3.0	-15	298	10

## Nitroethane

Formula:  $\text{CH}_3\text{CH}_2\text{NO}_2$

CAS Registry number: 79-24-3

NBS identification number: 622.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich 13,020-6, which was stated by the manufacturer to have been analyzed by gas-chromatography and infrared methods. Gas chromatography on a Chromosorb 102 column showed three impurities of 0.01, 0.97, and 3.64 percent. The sample was therefore purified on Chromosorb 102 before use.

Remarks.- The lines are exceptionally broad, and the frequencies and intensities are quite pressure sensitive. Few widths were measured at a pressure of 12 millitorr; attempts to remeasure the lines at 5 millitorr showed that many widths were still too large to measure, and the intensities of many of the lines dropped below threshold value.

The pressure of 12 millitorr was registered by a thermocouple gage as 37 millitorr.



NAME: NITROETHANE						ID NO. 622.00		
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
30941.13	.20	66		1	3.85	-18	297	12
30964.06	.10	64		1	2.65	-18	297	12
30975.47	.10	65		1	2.65	-17	297	12
30980.89	.10	66		1	2.15	-18	297	12
30982.86	.10	66		1	2.15	-18	297	12
31020.31	.10	66		1	3.4	-18	297	12
31023.29	.10	64		1	3.4	-18	297	12
37720.07	.10	64		1	3.05	-17	297	12
38323.22	.20	66	48	3	3.0	-16	297	12
38413.217	.05	66	47	4	3.4	-16	297	12
38548.68	.10	64		1	3.45	-16	297	12
38621.01	.10	64		1	2.65	-16	297	12
38624.80	.10	63		1	3.85	-16	297	12
38654.98	.10	65		1	1.7	-16	298	12
38662.08	.10	64		1	3.45	-16	298	12
38668.08	.10	63		1	3.0	-16	298	12
38683.75	.10	64		1	3.45	-16	298	12
38687.26	.10	64		1	2.6	-16	298	12
38694.28	.10	65		1	2.15	-16	298	12
38702.09	.10	65		1	3.8	-16	298	12
38705.53	.10	65		1	2.1	-16	298	12
38714.82	.10	62		1	3.0	-16	298	12
38724.06	.10	63		1	3.45	-16	298	12
38729.18	.10	63		1	3.05	-16	298	12

## Nitromethane

Formula:  $\text{CH}_3\text{NO}_2$

CAS Registry number: 75-52-5

NBS identification number: 550.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Fisher N-98 Certified reagent. Chromatography on a Chromosorb 102 column showed impurities of 0.15, 0.26, 3.1, and 1.3 percent. The sample was therefore purified on a Chromosorb 102 column before using.

Remarks.- The sample was initially run at a pressure of 10 millitorr, but the lines were so broad that it was rerun at 5 millitorr. The frequencies and/or intensities may be pressure sensitive because of the unresolved overlaps.

The sample identity has been confirmed by matching 13 of the lines to reported  $J = 1 - 2$  transitions (ref. 3).

A sample pressure of 10 millitorr was registered as 23 millitorr by a thermocouple gage, and the pressure of 5 millitorr was registered as 11 millitorr.

NAME: NITROMETHANE					ID NO. 550.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
28267.905	.02	65	47	4	3.0	-16	296	5
29571.685	.01	56.7	37.7		3.0	-18	296	5
30037.357	.02	59	40	4	2.1	-18	296	5
30255.99	.20	61	40	5	2.1S	-18	297	5
30788.61	.20	59	40	6	2.1S	-18	297	5
31053.12	.20	64	45	3	2.6	-17	297	5
31426.844	.05	65	46	4	1.7	-18	297	5
31677.440	.05	61	41	4	1.7	-18	297	5
31802.65	.20	59	38	6	2.1S	-18	297	5
31893.81	.10	65		1	2.1S	-18	297	10
31989.287	.02	63	45	5	2.1	-18	297	5
32034.31	.20	62	41	5	2.1S	-18	297	5
32190.002	.02	62	41	5	2.1	-18	297	5
32345.547	.02	58	40	4	2.1	-18	297	5
32578.796	.02	64	43	5	3.8	-18	298	5
32586.630	.05	62	42	4	1.7	-18	296	5
32660.01	.20	64	43	4	2.1S	-17	297	5
32690.41	.10	65		1	2.1S	-18	298	10
32801.065	.02	66	47	5	2.1	-17	299	10
32826.955	.02	59.4	39.5		2.1	-18	297	5
32858.240	.02	60.4	40.7		2.1	-17	297	5
32959.848	.01	58.5	38.7		3.4	-17	297	5
32983.12	.20	64	43	5	2.1S	-17	297	5
33389.24	.20	61	40	4	2.1S	-17	297	5
33476.818	.02	61	41	5	3.4	-17	297	5
33643.89	.20	61	41	5	2.1S	-17	297	5
33909.606	.05	65	46	4	1.7	-18	297	5
33929.477	.05	65	47	4	3.0	-17	298	10
33988.932	.02	61	41	4	2.1	-17	297	5
34002.69	.20	57	37	6	2.1S	-18	297	5
34040.485	.02	65	47	4	3.0	-18	297	5
34404.40	.20	57	38	6	2.1S	-17	297	5
34523.53	.20	63	45	4	2.1S	-17	297	5
35321.40	.20	63	42	5	2.1S	-17	298	5
35516.39	.20	57	37	6	2.1S	-17	298	5
35550.92	.10	65	47	5	1.7S	-17	298	5
35655.489	.01	54.9	36.1		2.1	-17	297	5
36433.69	.20	65	46	3	2.1S	-16	298	5
37040.005	.02	66	48	4	2.1	-15	298	5
37061.687	.01	57.5	39.4		2.1	-15	296	5
37658.848	.02	66	47	5	1.7	-17	296	5
38333.173	.02	65	47	5	3.8	-16	297	10
38681.18	.10	62	41	4	1.7	-16	296	5
38812.552	.02	65	47	5	2.1	-15	298	10
39226.47	.20	62	42	3	2.1S	-15	297	5
39254.29	.10	66		1	2.6S	-15	298	10
39318.80	.20	63	42	4	2.1S	-15	297	5
39330.42	.20	60	39	4	2.1S	-15	297	5
39531.59	.20	59	39	6	2.1S	-14	297	5
39642.168	.05	66	48	4	2.1	-14	298	10

NAME: NITROMETHANE			CONT INUED			ID NJ. 550.00		
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
39804.369	.02	65	46	4	1.7	-15	297	5
39917.793	.01	59.0	41.4		2.1	-15	297	5

## Propanenitrile

Formula:  $\text{CH}_3\text{CH}_2\text{CN}$

CAS Registry number: 107-12-0

Synonyms: ethyl cyanide, propionitrile

NBS identification number: 419.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman P528. Chromatography on a Chromosorb 102 column showed a water impurity of about 0.5 percent and one other impurity of 0.1 percent.

Remarks.- The water content of the sample was reduced by distilling the sample into the cell at low temperature.

The lines of propanenitrile are exceptionally broad and most of them exhibit some degree of asymmetry. The original measurements were made at 10 millitorr, but the pressure was reduced to 5 millitorr to improve accuracy. Even at that low pressure the line widths are of the order of 0.5 MHz.

Most of the lines have been verified by matching them with their theoretically assigned transitions (ref. 3). In addition, data from both older spectrometers were available for comparison.

NAME: PROPANENITRILE					ID NO. 419.00			
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26817.821	.02	57.3	37.4		1.7	-20	296	5
26829.260	.05	62	42	4	3.0	-19	296	5
26848.92	.20	63	41	2	2.6	-19	296	5
26860.457	.05	61	41	4	3.4	-19	297	5
26878.49	.20	63		1	1.75	-20	297	5
26890.13	.10	65	43	4	2.1	-19	297	5
26988.635	.05	64	45	4	1.7	-19	297	5
27561.76	.20	58	37	3	1.7	-19	297	5
27592.230	.05	62	42	4	2.6	-18	297	5
28622.276	.05	63	44	4	2.6	-18	297	5
34824.039	.01	53.8	34.3		2.1	-16	297	5
34897.721	.02	58.0	38.5		2.1	-16	297	5
35722.205	.02	53	34	4	1.7	-16	297	5
35742.468	.05	58	38	4	2.1	-16	297	5
35776.55	.10	58	38	6	2.15	-16	297	5
35792.18	.10	56	35	4	1.7	-16	297	5
35806.36	.10	63	42	4	2.1	-16	297	5
35813.94	.20	58		1	2.15	-16	297	5
35814.87	.20	56	35	2	2.65	-16	298	5
35831.77	.20	61	40	2	3.05	-16	298	5
35844.62	.20	60	39	2	2.6	-16	298	5
35862.54	.20	61	38	2	2.15	-16	298	5
35866.25	.10	56	34	4	2.1	-16	298	5
35871.74	.10	64	43	4	2.1	-16	298	5
36739.664	.02	53.4	33.9		3.0	-16	298	5

## 2-Propenenitrile

Formula:  $\text{CH}_2\text{:CHCN}$

CAS Registry number: 107-13-1

Synonyms: acrylonitrile, vinyl cyanide

NBS identification number: 223.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman P5161 which was stated to be inhibited by about 40 ppm of p-methoxyphenol. Chromatography on a Porapak N column showed only a single impurity of about 0.6 percent, which appeared to be water.

Remarks.- The first scan was made at a pressure of 9 millitorr. Because the lines are so broad, most of the stronger ones were also measured at 5 millitorr to improve the accuracy. The 9-millitorr measurements are given only for those lines which were not remeasured.

Sample identity was confirmed by matching five observed lines with the theoretically calculated transitions (ref. 3). Data were also compared with a recording of the spectrum made on the Tracerlab spectrometer.

The operating pressure of 9 millitorr was registered as 22 millitorr by a thermo-couple gage.

NAME: 2-PROPENENITRILE						ID NO. 223.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
27767.400	.05	54	34	4	2.6	-18	298	5
27813.500	.05	61	41	4	2.1	-18	298	5
27833.184	.05	59	39	4	2.1	-18	298	5
28440.977	.02	53	34	4	2.1	-17	298	5
28457.28	.20	59		1	2.6S	-17	298	5
28471.07	.20	59	37	2	3.4S	-17	298	5
28478.521	.02	59.9	40.7		2.1	-17	298	5
28523.141	.05	58	39	4	2.6	-19	298	5
29139.150	.05	54	34	2	1.7	-19	298	5
29167.11	.20	61	41	2	2.6	-19	298	5
29239.159	.05	58	39	2	1.7	-18	298	5
29337.48	.05	64	44	5	2.1	-18	298	9
30943.52	.05	66	47	5	2.1	-17	298	9
31778.61	.05	64	45	5	2.1	-16	298	9
32420.45	.05	67	48	5	3.0	-15	298	9
33125.59	.10	66	47	5	2.6	-17	298	9
35396.40	.05	66	49	5	3.4	-16	299	9
35563.96	.05	64	46	5	3.0	-16	299	9
35827.75	.10	64	46	5	3.4	-16	299	9
36330.75	.10	67	48	5	2.6	-15	300	9
36535.15	.05	64	47	5	2.1	-16	300	9
36977.89	.05	62	43	5	1.7	-15	300	9
36995.35	.10	63	44	5	2.6	-15	300	9
37018.923	.02	49.9	31.0		2.6	-16	298	5
37057.47	.05	64	46	5	2.1	-16	300	9
37064.56	.10	66	48	5	1.7	-16	300	9
37080.588	.02	56.5	37.8		2.1	-17	298	5
37106.374	.01	54.2	35.5		2.1	-17	298	5
37159.04	.10	62	44	5	1.7	-16	300	9
37191.951	.02	59.2	40.5		2.1	-16	298	5
37851.441	.05	60	42	4	2.1	-16	298	5
37904.853	.01	48.7	30.3		2.1	-17	298	5
37914.43	.20	64		1	1.7	-16	300	9
37939.818	.05	51	32	2	1.7	-17	298	5
37952.99	.20	52	31	2	2.1S	-17	298	5
37955.539	.02	55	36	4	2.1	-17	297	5
37959.68	.20	63	46	2	2.1	-15	295	9
37964.85	.20	67		1	2.1	-15	295	9
37974.49	.20	52	32	2	2.6	-18	297	5
38002.43	.20	59	38	4	2.1S	-17	297	5
38013.315	.01	53.3	34.9		2.6	-17	297	5
38022.45	.20	59	39	2	2.6	-17	297	5
38039.23	.20	65	46	3	1.7	-15	295	9
38050.14	.10	57	36	2	2.1	-17	297	5
38063.65	.20	57	36	2	2.1S	-17	297	5
38070.57	.20	64		1	1.7	-15	296	9
38087.16	.20	57	37	2	2.1	-17	297	5
38097.87	.20	63		1	1.7	-15	296	9
38111.88	.20	64		1	2.1	-15	296	9
38119.722	.01	57.9	39.1		2.6	-18	297	5



NAME: 2-PROPENITRILE

CONTINUED

ID NO. 223.00

$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
38133.49	.20	63	43	2	2.1	-15	296	9
38158.48	.20	61	42	2	2.15	-18	298	5
38172.27	.20	62		1	2.1	-15	297	9
38179.67	.10	65	46	5	2.6	-15	297	9
38190.39	.10	63	44	5	2.6	-15	297	9
38197.78	.20	61	42	5	1.7	-16	297	9
38223.96	.05	63	45	5	3.4	-16	297	9
38306.38	.10	66	47	5	2.1	-16	297	9
38740.68	.05	61	44	5	1.7	-15	297	9
38847.736	.02	49.2	30.3		2.1	-16	298	5
38878.06	.20	64	47	2	1.7	-15	297	9
38885.225	.01	56.3	37.5		1.7	-17	298	5
38923.20	.05	63	45	5	2.1	-15	297	9
38980.806	.02	54.1	35.3		2.1	-17	298	5
39014.470	.02	61	42	4	1.7	-17	298	5
39111.687	.02	58.7	40.0		1.7	-17	298	5
39240.28	.10	63	45	5	2.1	-15	297	9

## 2-Propene-1-thiol

Formula:  $\text{CH}_2\text{:CHCH}_2\text{SH}$

CAS Registry number: 870-23-5

Synonym: allyl mercaptan

NBS identification number: 713.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich 12,280-7, which was stated by the manufacturer to have undergone analyses by elemental, infrared, and gas-chromatography methods. The purity was given as at least 70 percent, with the remainder being allyl disulfide. However, chromatography on a Chromosorb 102 column showed only two impurities of 0.1 percent and one of 0.6 percent.

Remarks.- Two weak lines were observed which could be almost completely eliminated by distilling the sample into the cell at low temperature. Sample identity was confirmed by the observation of seven theoretically verified lines (ref. 6).

The sample pressure of 15 millitorr was registered as 45 millitorr by a thermocouple gage.

NAME: 2-PROPENE-1-THIOL						ID NO. 713.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
27475.813	.02	65	52	5	3.8	-17	298	15
32693.244	.02	64	52	4	3.4	-17	298	15
32966.21	.10	64	51	2	3.4	-17	297	15
32987.86	.10	63	51	4	2.15	-17	297	15
37293.324	.02	65	53	5	3.0	-14	298	15
38140.090	.02	63	51	4	3.8	-16	297	15
38454.039	.01	62	50	5	3.8	-15	297	15
38475.805	.02	64	51	4	3.8	-16	297	15
38485.83	.10	62	49	4	3.85	-15	297	15
38489.93	.20	62	50	3	3.85	-15	297	15
38523.89	.10	64	51	5	3.85	-14	298	15
38802.830	.01	63	50	5	3.0	-15	298	15

## Pyridine

Formula: N:CHCH:CHCH:CH

CAS Registry number: 110-86-1

NBS identification number: 235.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The same was Fisher Certified P-368. Chromatography on a Chromosorb 102 column showed three impurity peaks of less than 0.1 percent each.

Remarks.- Some lines could not be completely modulated with the maximum available field of 3.8 kV/cm. Others may be undermodulated at the field used because the higher fields resulted in interference by Stark lobes from adjacent lines.

Sample identity was confirmed by matching 16 of the observed lines with the theoretical transitions (ref. 3). Data were also compared with a recording of the spectrum made on the Hewlett-Packard 8400B spectrometer.

The 10-millitorr pressure was registered as 30 millitorr on a thermocouple gage.

NAME: PYRIDINE					ID NO. 235.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26515.655	.02	66	50	5	1.7	-19	298	11
26519.93	.10	61	46	3	2.1	-19	298	10
26524.845	.02	65	48	5	2.1	-19	298	10
26540.44	.10	59	43	3	3.4	-19	298	10
26548.85	.10	61	46	2	3.4	-19	298	10
26559.51	.10	65	50	2	1.7	-19	298	10
26569.49	.10	59	43	3	3.0	-19	298	10
26577.35	.10	61	46	3	2.6	-19	298	10
26595.816	.05	64	48	4	1.7	-19	298	10
26597.657	.02	67	51	5	1.7	-19	298	10
26604.97	.10	61	45	3	2.6	-19	298	10
26623.53	.10	63	47	3	3.0	-19	298	10
26624.262	.05	62	1	1	3.0	-19	298	10
26632.20	.10	67	52	3	2.6	-18	298	10
26634.57	.10	56	41	2	3.8	-19	298	10
26636.619	.05	64	49	4	2.1	-19	298	10
26637.69	.10	66	51	2	2.1	-19	298	10
26649.42	.10	65	50	3	3.4	-19	299	10
26652.98	.10	65	50	2	2.1	-19	299	10
26775.519	.02	58	41	4	3.0	-20	298	10
26926.132	.05	61	45	4	2.1	-19	298	10
27032.084	.02	59	42	4	2.1	-21	298	10
27033.18	.20	62	46	2	2.6	-21	298	10
27235.261	.02	57	40	4	2.1	-20	298	10
27705.41	.10	61	46	2	2.1	-17	297	10
27739.59	.10	60	44	2	1.7	-17	297	10
27748.42	.10	59	44	2	2.1	-17	297	10
27787.93	.10	56	40	2	2.1	-17	297	10
27930.25	.20	59	43	3	2.1	-17	297	10
28017.39	.20	65	49	3	2.1	-16	297	10
28629.09	.20	64	48	2	1.7	-17	297	10
28888.09	.10	58	42	2	3.0	-16	297	10
28919.74	.10	57	41	3	2.1	-16	297	10
29275.371	.02	62	46	4	2.1	-16	297	10
29531.78	.10	58	43	2	3.0	-16	297	10
29674.42	.10	56	40	2	2.1	-16	297	10
29769.158	.02	55	39	4	3.0	-16	297	10
29933.543	.02	63	46	4	2.6	-16	297	10
30236.17	.10	57	41	2	2.1	-16	297	10
30262.21	.10	60	44	3	1.7	-16	297	10
30366.42	.10	64	48	2	2.1	-16	297	10
30456.890	.02	57	41	4	3.0	-16	297	10
30886.59	.20	64	48	2	2.1	-15	297	10
30983.521	.02	54.2	38.4	3	3.8	-19	297	10
31001.83	.10	62	47	2	1.7	-19	297	10
31038.812	.02	62	47	4	2.1	-19	297	10
31255.945	.02	62	47	4	3.0	-19	297	10
31268.67	.20	64	46	3	3.0	-19	297	10
31358.27	.10	58	42	2	2.1	-18	297	10
31381.873	.01	56.3	40.8	3	3.8	-18	297	10

NAME: PYRIDINE		CONTINUED				ID NO. 235.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	P, mtorr
31629.805	.02	63	47	5	1.7	-19	297	10
31644.653	.02	62	46	5	1.7	-19	297	10
31672.694	.02	60	43	4	1.7	-19	297	10
31681.465	.02	55	40	4	2.1	-19	297	10
31694.046	.01	56.2	40.6		3.4	-19	297	10
31698.170	.02	54	38	4	2.6	-19	297	10
31756.927	.02	57	41	4	3.0	-19	297	10
31775.331	.01	54.1	38.3		2.6	-19	297	10
31806.29	.10	61	46	3	3.8	-19	294	10
31846.798	.01	53.7	38.3		3.4	-18	297	10
31860.499	.05	62	46	4	3.4	-18	297	10
31861.85	.10	61	45	3	2.6	-18	297	10
31862.90	.20	61	45	2	2.1	-18	297	10
31906.768	.02	57	42	4	3.8	-18	297	10
31942.221	.02	61	45	5	1.7	-18	297	10
31950.593	.02	55.9	40.2		3.4	-19	295	11
31968.39	.10	63	47	3	3.8	-19	295	10
31969.71	.10	64	48	2	3.4	-19	295	10
31980.762	.02	56.4	40.3		2.1	-18	295	10
32007.95	.10	58	42	3	2.1	-18	297	10
32012.694	.02	62	46	4	3.4	-18	295	10
32056.334	.02	54	38	4	3.8	-18	295	10
32071.496	.05	62	46	4	2.6	-18	296	10
32076.790	.05	55	41	4	3.8	-18	296	10
32119.482	.02	63	47	4	3.8	-18	296	10
32138.349	.02	63	47	5	1.7	-18	296	10
32156.204	.01	56.2	40.7		3.0	-18	296	10
32160.55	.10	63	47	3	1.7	-18	296	10
32161.09	.10	61	48	2	1.7	-18	296	10
32194.309	.05	61	45	4	3.4	-18	296	10
32205.572	.02	57	42	4	3.8	-18	296	10
32245.724	.01	54.2	38.7		3.8	-18	296	10
32250.922	.05	63	47	4	2.6	-18	296	10
32267.485	.02	65	49	4	2.6	-18	296	10
32303.572	.02	54	39	4	3.8	-19	296	10
32322.737	.02	56.7	41.2		3.4	-19	296	10
32328.103	.02	62	47	5	3.8	-19	296	10
32357.322	.02	54	38	4	2.6	-18	296	10
32361.326	.02	63	46	5	3.8	-18	296	10
32378.193	.01	56.9	40.8		3.8	-18	296	10
32386.769	.02	55	39	4	3.8	-18	296	10
32389.08	.20	62	45	2	3.8	-18	296	10
32415.001	.05	64	48	4	2.1	-18	297	10
32434.821	.05	55	40	4	2.6	-19	297	10
32438.372	.05	58	42	4	3.4	-19	297	10
32443.812	.05	63	46	4	3.0	-19	297	10
32478.729	.05	56	39	4	3.8	-19	297	10
32509.272	.05	56	38	4	3.8	-19	296	10
32523.71	.10	58	42	2	3.0	-19	296	10
32527.60	.10	57	42	2	2.6	-19	296	10

NAME: PYRIDINE		CONTINUED				ID NO. 235.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
32531.81	.10	57	42	3	2.6	-19	296	10
32547.680	.05	58	42	4	3.0	-19	296	10
32548.38	.10	60	46	2	2.6	-19	296	10
32552.659	.01	52.1	37.2	3	3.4	-17	297	10
32573.423	.02	61	46	4	2.6	-19	296	10
32577.320	.05	60	46	4	2.1	-19	296	10
32593.00	.10	59	44	2	2.6	-19	296	10
32787.446	.05	54	38	4	3.0	-19	296	10
32959.59	.20	57	41	3	2.1	-19	296	10
33051.77	.20	64	47	3	1.7	-18	296	10
33221.121	.05	62	45	4	3.0	-17	297	10
33409.56	.10	63	47	3	3.0	-17	297	10
33635.378	.05	63	46	4	1.7	-18	297	10
33847.83	.20	55	39	3	2.1	-17	297	10
33967.63	.20	56	40	2	3.4	-19	297	10
34184.77	.10	58	43	2	3.0	-18	297	10
34192.033	.05	60	44	4	3.4	-18	297	10
34192.98	.20	62	46	2	3.8	-18	297	10
34290.287	.05	64	47	4	2.6	-18	297	10
34562.47	.10	55	39	2	2.0	-18	297	10
34919.853	.02	53	37	4	3.4	-18	297	10
35016.520	.02	62	46	4	3.0	-17	297	10
35022.73	.10	57	41	2	3.0	-17	297	10
35083.82	.10	58	42	3	2.1	-18	297	10
35149.124	.02	61	45	4	3.0	-18	297	10
35407.31	.10	63	47	2	3.0	-18	297	10
35445.401	.02	62	46	5	2.6	-18	297	10
35668.66	.10	62	48	2	2.6	-17	297	10
35674.892	.02	55.0	39.0	3	3.0	-17	296	10
35756.08	.10	63	47	2	2.6	-17	296	10
35829.134	.02	63	47	4	3.4	-17	296	10
36267.198	.02	53	37	4	3.8	-17	296	10
36329.99	.10	56	41	2	3.0	-17	296	10
36363.280	.02	60	45	4	2.6	-17	296	10
36563.740	.02	61	46	5	3.0	-16	296	10
36724.64	.10	56	40	3	2.1	-16	296	10
36729.989	.02	54.5	38.9	3	3.8	-17	296	10
36782.046	.02	62	47	5	3.8	-16	296	10
36829.006	.02	59	43	4	2.1	-17	296	10
36830.10	.10	61	45	2	1.7	-17	296	10
36835.47	.10	62	48	2	3.4	-17	296	10
36838.567	.02	62	46	4	3.4	-17	296	10
36846.883	.02	60	44	4	2.1	-16	296	10
36868.305	.02	63	48	5	2.1	-16	297	10
36873.577	.05	63	48	4	2.1	-16	297	10
36891.082	.02	63	47	4	2.1	-16	297	10
36927.526	.01	54.8	39.4	3	3.8	-16	297	10
36939.340	.01	52.9	37.2	3	2.1	-16	297	10
36954.529	.02	60.3	44.9	3	2.6	-16	297	10
36994.287	.01	52.6	37.2	3	3.4	-16	297	10

NAME: PYRIDINE			CONTINUED			ID NO. 235.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
36999.608	.02	61	45	4	2.6	-16	297	10
37012.106	.05	64	47	4	2.6	-16	297	10
37035.922	.02	62	46	5	1.7	-16	297	10
37066.683	.01	55.1	39.5		2.1	-16	297	10
37080.247	.02	62	47	5	3.0	-17	297	10
37092.191	.02	53	38	4	3.4	-17	297	10
37110.493	.02	54	38	4	3.8	-17	297	10
37135.665	.02	61	46	5	1.7	-17	297	10
37183.65	.10	60	45	2	2.1	-17	297	10
37226.337	.02	60	45	4	2.6	-17	297	10
37253.925	.01	52.2	36.8		3.0	-17	297	10
37294.370	.02	61	46	4	2.1	-17	297	10
37354.743	.01	53.4	37.5		2.6	-18	297	10
37373.926	.02	62	47	4	2.1	-18	297	10
37377.291	.02	55	40	4	3.8	-18	297	10
37408.343	.01	54.3	38.9		3.8	-17	297	10
37419.14	.10	58	42	2	3.4	-17	297	10
37450.222	.02	63	48	4	2.1	-17	296	10
37528.550	.01	59.8	44.3		3.8	-17	296	10
37562.345	.01	52.3	36.7		3.8	-17	296	10
37599.205	.02	61	45	4	3.8	-17	296	10
37708.510	.02	54	39	4	3.8	-18	296	10
37784.981	.05	55	41	4	3.8	-18	297	10
37786.03	.20	62	46	2	2.6	-18	297	10
37787.56	.20	62	45	3	2.1	-18	297	10
37796.583	.02	60	45	4	3.4	-18	297	10
37823.108	.05	54	37	4	3.0	-18	297	10
37842.328	.02	52	37	4	3.8	-18	297	10
37856.888	.02	56.3	40.6		2.1	-18	297	10
37858.776	.02	61	45	4	3.0	-18	297	10
37884.327	.05	61	46	4	3.8	-18	297	10
37909.758	.02	62	47	4	3.9	-17	297	10
37931.325	.02	53	38	4	3.8	-17	297	10
37944.069	.02	62	46	4	2.1	-17	297	10
37948.88	.10	61	47	3	3.4	-17	297	10
37961.532	.01	54.7	39.7		3.8	-17	297	10
38008.092	.02	60	45	4	3.8	-17	297	10
38050.156	.02	55	40	4	3.8	-17	297	10
38057.339	.05	61	46	4	3.8	-17	297	10
38065.421	.02	52	37	4	3.8	-17	297	10
38085.812	.02	61	45	4	3.8	-17	297	10
38130.749	.02	62	47	4	3.0	-17	297	10
38146.906	.02	53	38	4	2.8	-17	297	10
38154.260	.02	55	39	4	3.8	-17	297	10
38159.709	.05	63	48	4	2.6	-17	297	10
38162.495	.02	61	46	5	3.8	-17	297	10
38172.156	.02	62	46	4	1.7	-17	297	10
38198.304	.02	62	47	4	3.8	-17	296	10
38225.629	.05	56	41	4	2.0	-17	296	10
38228.990	.02	53	38	4	3.8	-17	296	10



NAME: PYRIDINE			CONTINUED			ID NO. 235.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
38268.32	.20	61	45	2	3.8	-17	297	10
38289.426	.05	54	39	4	3.8	-18	297	10
38290.853	.02	55	40	4	3.8	-18	297	10
38292.05	.20	60	43	2	3.8	-18	297	10
38306.404	.02	60	45	4	3.8	-18	297	10
38324.96	.10	62	47	3	3.8	-17	297	10
38336.521	.05	62	46	4	3.4	-17	297	10
38341.25	.20	53	37	2	3.8	-17	297	10
38350.36	.10	62	47	3	3.8	-17	297	10
38355.66	.10	61	46	2	2.6	-17	297	10
38359.69	.10	62	47	3	3.8	-17	297	10
38369.30	.10	61	45	3	3.4	-17	297	10
38377.59	.10	63	48	2	2.6	-18	297	10
38381.628	.02	52	36	4	3.8	-17	298	10
38413.56	.10	53	37	3	3.8	-17	298	10
38438.14	.10	53	38	3	3.8	-17	298	10
38456.68	.10	55	39	3	3.8	-17	298	10
38465.600	.02	61	45	5	2.1	-17	298	10
38467.214	.02	62	47	4	2.6	-17	298	10
38470.989	.01	48.9	33.8		3.8	-17	297	10
38473.63	.10	54	40	2	2.6	-17	298	10
38477.10	.10	57	42	2	3.8	-17	298	10
38497.223	.02	58	43	4	3.8	-17	298	10
38501.799	.01	57.2	42.5		3.0	-17	298	10
38532.339	.05	62	47	4	3.0	-17	298	10
38633.241	.05	54	38	4	2.6	-17	298	10
38651.004	.05	62	46	4	3.0	-17	298	10
38815.303	.05	59	43	3	2.6	-17	296	10
38816.02	.10	61		1	2.6	-17	296	10
38915.35	.10	64	49	2	2.6	-16	296	10
38970.50	.10	64	49	3	3.8	-16	296	10
38987.542	.05	56	40	4	2.6	-16	296	10
39013.32	.10	61	46	3	3.4	-16	297	10
39013.790	.05	59	44	2	3.4	-16	297	10
39056.464	.05	55	39	4	2.6	-16	297	10
39533.40	.10	55	40	2	3.4	-16	297	10
39719.502	.05	63	47	4	3.0	-16	297	10
39747.64	.10	57	41	3	2.6	-17	297	10
39911.443	.02	61	45	4	2.6	-17	297	10
39912.66	.20	63	47	2	2.6	-17	297	10
39938.95	.10	57	42	2	3.4	-18	297	10

## Pyrrole

Formula: NHCH:CHCH:CH

CAS Registry number: 109-97-7

Synonym: azole

NBS identification number: 764.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman P1331. Analysis with a Chromosorb 102 column showed impurities of 0.55, 0.03, 0.32, and 0.7 percent. One of these was much less volatile than pyrrole and was kept frozen. The others were reduced by successive vacuum distillations.

Remarks.- After the spectral measurements were completed, a spot check showed that two of the samples had impurities resulting in reduced intensities. The errors were near 0.3 and 1.25 dB, respectively, for all the lines checked in the two groups. Therefore, all the lines in those groups were corrected by 0.3 or 1.25 dB.

Sample identity was confirmed by matching four of the observed lines with the transition frequencies calculated from rotational constants given in reference 3.

The sample pressure of 10 millitorr was registered as 32 millitorr on a thermocouple gage.

NAME: PYRROLE

ID NO. 764.00

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26797.704	.02	65	51	4	2.1	-17	298	10
26862.913	.02	61	47	5	2.1	-18	298	10
26929.019	.02	65	51	5	2.1	-17	298	10
27054.186	.01	62	50	4	1.7	-18	298	10
27354.051	.01	54.9	40.7		2.1	-16	296	10
27361.623	.01	55	42	4	3.0	-17	297	10
27405.770	.01	56.5	42.2		2.1	-16	297	10
27749.174	.02	63	49	5	3.4	-17	297	10
28113.139	.02	65	51	4	2.6	-17	297	10
28160.235	.01	53.2	38.9		2.1	-18	298	10
28472.866	.02	65	51	5	3.4	-18	297	10
28587.513	.01	54.6	40.3		2.1	-18	297	10
28863.909	.01	54.4	40.2		2.1	-18	297	10
28892.358	.01	56.6	43.2		2.1	-18	297	10
29017.123	.01	58.9	46.1		2.1	-18	298	10
29017.97	.10	64	50	2	3.0	-18	298	10
29100.228	.02	63	49	5	2.1	-18	298	10
29123.656	.01	59.4	44.7		1.7	-19	298	10
29466.515	.01	51.6	37.3		2.1	-18	298	10
29548.124	.01	65	52	5	1.7	-18	298	10
29965.935	.01	56.5	42.1		2.1	-17	297	10
29972.526	.01	53.6	39.2		3.0	-19	297	10
30080.142	.02	62	48	5	2.1	-17	297	10
30160.861	.05	64	51	5	3.8S	-17	297	10
30273.331	.02	64	50	4	2.6	-17	297	10
30343.952	.01	53.1	39.8		2.1	-17	297	10
30389.047	.01	51.3	37.0		3.8	-17	297	10
30445.653	.02	64	50	5	2.6	-17	297	10
30725.120	.01	53.4	39.1		3.0	-17	297	10
30739.637	.02	62	48	5	2.1	-18	298	10
30939.496	.01	59.7	46.9		2.1	-19	298	10
30990.984	.01	51.2	36.8		3.0	-19	298	10
31151.579	.02	62	47	5	3.4	-18	298	10
31197.209	.01	53.6	39.1		3.8	-18	298	10
31354.082	.01	51	37	4	3.8	-18	298	10
31471.042	.05	55	42	4	3.8	-18	298	10
31489.47	.10	64	49	2	1.7	-18	298	10
31496.565	.02	64	49	4	3.0	-18	298	10
31518.833	.02	64	49	4	3.4	-18	298	10
31536.11	.10	59	44	3	3.8	-18	298	10
31536.48	.10	60	45	2	3.4	-18	298	10
31538.78	.10	61	47	2	2.1	-18	298	10
31544.944	.02	62	48	5	3.4	-18	298	10
31547.58	.10	64	50	3	2.6	-18	298	10
31551.577	.01	54.3	40.2		2.6	-18	298	10
31556.569	.01	51.7	37.2		3.8	-18	298	10
31559.685	.05	62	47	4	1.7	-18	298	10
31573.30	.10	61	47	2	1.7	-18	298	10
31585.403	.05	63	48	4	2.6	-18	298	10
31617.674	.02	55	40	4	3.4	-17	297	10

NAME: PYRROLE			CONTINUED			ID NO. 764.03		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
31649.190	.02	54	39	4	3.4	-18	297	10
31650.462	.01	51.3	36.9		1.7	-18	297	10
31656.280	.01	51.9	37.6		1.7	-18	297	10
31660.322	.05	53	38	4	3.8	-18	297	10
31664.987	.02	54	40	4	3.0	-18	297	10
31667.984	.01	55	40	4	2.1	-18	297	10
31681.402	.02	53	38	4	3.0	-18	297	10
31689.33	.10	57	43	2	3.8	-18	297	10
31694.653	.05	55	40	4	3.0	-18	298	10
31699.041	.01	51.1	36.8		2.1	-18	298	10
31704.306	.01	56.3	43.5		3.4	-18	298	10
31706.49	.10	54	40	2	3.8	-18	298	10
31708.43	.10	55	40	2	2.6	-18	298	10
31716.22	.10	57	43	2	2.1	-18	298	10
31723.63	.10	56	42	2	2.1	-18	298	10
31724.758	.05	57	42	6	1.75	-18	298	10
31727.561	.05	54	37	4	3.8	-18	298	10
31728.84	.10	59	44	2	3.8	-18	298	10
31732.206	.01	59.2	43.4		3.8	-18	298	10
31759.943	.01	53.3	38.9		3.0	-18	298	10
31806.233	.01	62	48	5	2.6	-18	298	10
31856.678	.01	51.2	36.8		2.1	-18	298	10
31969.959	.02	64	50	5	1.7	-18	298	10
31999.729	.01	53.3	39.0		2.1	-18	298	10
32009.771	.02	64	50	4	1.7	-18	298	10
32132.951	.02	65	51	5	1.7	-18	298	10
32144.806	.02	64	50	5	2.1	-18	298	10
32194.462	.02	62	48	4	3.4	-18	298	10
32201.165	.01	51.3	36.7		2.1	-18	298	10
32474.704	.01	53.4	39.1		3.0	-17	297	10
32492.999	.02	64	50	5	2.6	-18	297	10
32614.999	.02	64	50	4	1.7	-17	297	10
32716.060	.01	63	50	5	2.1	-18	297	10
32803.963	.01	57	44	4	3.8	-17	297	10
32835.641	.01	51.6	37.3		2.1	-17	297	10
32839.881	.02	64	50	5	1.7	-17	298	10
32880.206	.01	62	48	5	3.0	-17	298	10
32963.197	.01	52.2	38.5		3.0	-17	298	10
33300.747	.01	53.7	39.4		2.1	-17	298	10
33351.222	.01	57.0	42.6		2.1	-17	298	10
33371.937	.02	64	50	5	2.1	-17	298	10
33621.667	.02	65	51	5	3.0	-17	298	10
33887.997	.01	52	38	4	2.1	-18	298	10
33958.69	.10	65	50	3	2.6	-18	298	10
33985.014	.01	62	49	5	1.7	-17	298	10
34022.906	.01	62	50	5	3.0	-18	298	10
34112.840	.01	54.1	40.3		3.0	-18	298	10
34202.889	.01	59.6	45.0		2.1	-17	298	10
34594.149	.01	58.1	45.2		3.4	-17	298	10
34616.185	.01	54.2	40.1		3.4	-17	298	10

NAME: PYRROLE		CONTINUED				ID NO. 764.00		
$\nu_0$ , MHz	$U$ , MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	$P$ , dBm	$T$ , K	$P$ , mtorr
34727.753	.02	65	51	5	3.4	-17	298	10
34736.798	.02	65	51	5	3.8	-17	298	10
34864.250	.01	62	49	5	1.7	-16	297	10
35148.302	.01	51	37	4	3.0	-17	297	10
35171.420	.02	65	51	5	2.1	-17	297	10
35367.643	.01	54.9	40.6		2.1	-17	297	10
35504.207	.01	52	38	4	2.1	-17	297	10
35637.855	.02	66	52	5	2.6	-16	297	10
35644.574	.02	63	49	5	2.1	-17	297	10
35775.417	.01	64	50	5	2.1	-16	283	10
35946.667	.02	66	52	5	1.7	-16	297	10
36036.79	.10	65	51	2	2.1	-16	297	10
36067.826	.01	53.4	39.5		3.0	-16	297	10
36198.487	.01	64	51	5	3.0	-16	298	10
36295.090	.01	55.6	42.6		2.1	-16	298	10
36457.702	.02	64	51	5	3.0	-16	298	10
36570.478	.01	54.6	40.7		2.1	-16	298	10
36578.134	.01	61	48	5	3.0	-16	298	10
36724.924	.02	65	52	5	1.7	-16	298	10
36813.205	.02	64	50	5	2.1	-16	298	10
36872.928	.01	50.8	36.9		3.4	-16	298	10
37001.457	.02	62	48	4	2.1	-16	298	10
37276.087	.02	63	50	5	3.0	-16	298	10
37482.06	.10	65	51	3	2.6	-16	298	10
37482.74	.10	66	52	2	2.6	-17	298	10
37568.199	.01	52.7	38.8		3.0	-17	298	10
37599.755	.01	57.6	43.4		2.1	-17	298	10
37768.311	.02	64	50	4	3.8	-17	298	10
37831.874	.01	52.8	38.8		2.1	-17	298	10
37875.346	.01	61	47	5	3.0	-16	298	10
37893.599	.01	56.6	43.6		2.1	-16	297	10
37992.883	.02	63	50	5	2.1	-16	298	10
38052.859	.01	63	49	5	3.4	-17	297	10
38160.793	.01	50.0	36.0		3.0	-17	297	10
38282.315	.05	65	51	4	2.6	-16	297	10
38307.490	.01	60	48	5	2.1	-16	297	10
38383.873	.02	62	48	4	3.0	-16	297	10
38532.575	.02	65	51	5	2.1	-16	297	10
38584.496	.02	64	50	5	3.0	-16	297	10
38659.813	.01	52.1	38.0		3.0	-16	297	10
38713.934	.02	63	49	5	3.0	-15	297	10
38810.844	.01	60.3	46.5		3.4	-16	297	10
38932.022	.02	63	49	4	3.4	-15	297	10
38999.32	.10	65	50	3	3.4	-15	297	10
39072.94	.20	64	49	3	3.85	-15	298	10
39075.471	.01	49.8	35.7		3.4	-15	298	10
39165.955	.02	62	48	5	3.8	-15	298	10
39302.913	.01	55.1	41.3		2.1	-15	298	10
39369.057	.02	63	49	5	3.4	-15	298	10
39378.769	.01	53.8	40.6		2.1	-14	297	10

NAME: PYRROLE		CONTINUED					ID NO. 764.00	
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
39418.399	.01	52.3	38.0	5	3.0	-15	297	10
39429.188	.02	65	52		2.1	-15	297	10
39458.914	.01	60.1	46.2		3.4	-15	297	10
39531.293	.05	63	49	5	3.85	-15	297	10
39699.047	.01	49.1	34.9		3.8	-15	297	10
39809.182	.01	63	49	5	3.8	-15	297	10
39835.546	.02	64	50	4	3.8	-15	297	10
39894.475	.02	60	46	4	3.8	-15	297	10
39927.152	.01	52	37	4	3.8	-15	297	10
39956.420	.02	60	45	4	1.7	-15	297	10

## Sulfur dioxide

Formula: SO<sub>2</sub>

CAS Registry number: 7446-09-5

NBS identification number: 66.00

Frequency range: 18 000 to 40 000 MHz

Sample.- The sample was Matheson anhydrous grade bottled gas with a stated purity of 99.98 percent. Chromatography on a Chromosorb 102 column showed no impurities.

Remarks.- The spectrum of sulfur dioxide has been extensively studied. Sample identity was confirmed by matching four of the lines to theoretical transitions (ref. 3). Many of the other lines have also been verified by using the data from numerous articles in the scientific literature. In addition, data were compared with measurements on both the other spectrometers.

Data below 26 500 MHz do not include information on Stark sensitivity or power level; however, the power was generally less than -15 dBm.

NAME: SULFUR DIOXIDE						ID NO. 66.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
19637.11	.10	56	44	4	2.1		299	15
20335.40	.02	52	39	7	2.1		299	15
22065.68	.05	62	50	4	2.1		299	15
22220.36	.02	63	51	7	2.1		299	15
22482.56	.02	51	39	7	3.0		299	15
22733.96	.02	62	50	7	2.1		299	14
22904.90	.02	62	49	7	2.1		299	14
22928.57	.02	63	51	7	2.1		299	14
23034.81	.02	56	44	7	2.1		299	14
23414.24	.02	52	40	7	2.1		299	14
23732.98	.02	63	51	7	2.1		299	14
24039.63	.02	50	38	7	2.1		299	14
24083.47	.02	52	40	7	2.6		299	14
24319.65	.02	58	46	7	2.1		299	14
24834.26	.02	54	52	7	2.1		299	14
25049.45	.02	54	42	7	2.1		299	14
25392.82	.02	50	38	7	2.1		299	14
26411.48	.02	61	49	7	2.1		299	14
26776.592	.01	47.9	35.2		2.1	-18	293	15
26850.280	.02	60.2	47.9		3.0	-18	293	15
27932.420	.01	52.7	40.2		3.8	-17	293	15
28138.394	.01	56.7	44.9		3.0	-17	293	15
28173.485	.02	60.3	48.0		2.1	-17	293	15
28858.019	.01	47.4	34.8		3.0	-18	293	15
29052.079	.01	58.0	45.4		2.1	-18	293	15
29321.528	.01	45	34	4	3.8	-18	293	15
30205.545	.01	53.1	40.6		3.0	-18	293	15
30975.419	.01	59.3	47.1		1.7	-18	293	15
31089.924	.01	55.3	42.5		3.4	-18	293	15
31922.281	.01	46	33	4	2.1	-18	293	15
32214.670	.01	60.1	47.9		2.1	-18	293	15
33212.805	.01	60.1	47.6		3.0	-17	293	15
34097.746	.01	46.8	34.3		2.1	-18	293	15
34393.567	.01	57.8	46.3		2.1	-18	293	15
34425.15	.05	67		1	2.1	-18	293	15
34462.35	.05	72		1	2.1	-18	293	15
34530.203	.01	58.6	46.1		2.1	-18	293	15
34810.948	.01	63	51	5	1.7	-18	293	15
34971.637	.01	56.6	44.1		2.1	-18	293	15
35855.889	.02	63	50	5	3.4	-16	293	15
36065.277	.01	47.8	35.5		3.0	-16	293	15
36338.100	.01	46.9	34.4		2.1	-16	293	15
36791.049	.01	59.9	47.6		3.8	-16	293	15
36857.021	.01	57.0	44.4		2.1	-16	293	15
37351.807	.01	44.9	32.3		3.0	-16	293	15
37525.207	.01	61	49	5	1.7	-16	293	15
38518.224	.01	44.3	31.6		2.1	-16	293	15
38909.706	.01	54.6	42.1		3.8	-15	293	15
39447.007	.01	53.2	41.3		2.1	-15	293	15



## Tetrahydrothiophene

Formula: SCH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>CH<sub>2</sub>

CAS Registry number: 110-01-0

NBS identification number: 805.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich T1,560-1 with a stated purity of greater than 93 percent. Sample identity was verified by the manufacturer by gas chromatography and infrared and elemental analyses. Chromatography on a Chromosorb 102 column showed two impurities of 0.02 percent or less and one of 1.3 percent.

Remarks.- Some of the lines were less than 300 kHz wide. However, most were wider and many exhibited some asymmetry. It is therefore likely that some of the frequencies and/or intensities may be pressure sensitive because of overlaps.

The sample pressure of 15 millitorr was registered as 50 millitorr by a thermocouple gage.

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
26625.884	.05	64	49	4	2.1	-18	297	15
27044.373	.02	64	50	4	2.1	-17	298	15
27534.453	.02	64	49	4	2.1	-17	298	15
27972.683	.05	64	50	4	3.8	-18	298	15
28118.149	.02	63	48	4	2.1	-17	298	15
28404.445	.02	65	50	5	2.1	-18	298	15
28838.330	.02	63	49	5	3.8	-18	298	15
29012.041	.02	64	50	5	3.4	-18	298	15
29236.813	.02	65	50	5	3.8	-18	298	15
29721.856	.02	65	51	5	1.7	-18	298	15
29728.945	.02	63	49	4	2.1	-18	298	15
29802.561	.02	65	51	5	3.8	-18	298	15
30032.324	.02	65	50	5	1.7	-18	297	15
30239.372	.02	61	47	5	2.1	-17	297	15
30244.526	.02	64	50	4	2.1	-17	297	15
30295.328	.02	61	46	5	3.0	-17	297	15
30300.877	.02	64	50	5	2.6	-18	297	15
30566.553	.02	63	49	5	2.1	-17	297	15
30791.744	.05	64	49	4	2.6	-17	297	15
31399.168	.02	66	51	5	2.6	-18	297	15
31515.677	.02	65	50	4	2.1	-18	297	15
31560.386	.02	64	49	5	2.6	-18	298	15
31757.693	.05	65	51	4	3.4	-18	298	15
31899.220	.02	66	51	5	3.8	-18	298	15
31983.370	.05	64	49	4	3.0	-18	298	15
31992.570	.02	63	48	5	3.0	-18	298	15
32204.735	.02	65	51	4	2.6	-18	298	15
32233.047	.02	63	48	5	2.1	-18	298	15
32974.730	.02	64	50	5	3.4	-17	298	15
33465.348	.02	65	50	5	2.1	-17	298	15
33841.072	.02	63	48	5	2.1	-18	298	15
34018.69	.20	62	48	2	3.0	-18	298	15
34318.927	.02	64	50	5	3.8	-17	298	15
34323.901	.05	62	47	4	3.8	-18	298	15
34621.664	.02	65	52	5	2.1	-17	296	15
34973.707	.02	65	50	4	2.6	-17	296	15
35267.820	.02	63	49	4	3.8	-17	297	15
35295.693	.02	65	52	4	1.7	-17	297	15
35300.561	.02	60.2	45.5	5	3.0	-17	298	15
35393.398	.02	62	47	5	3.0	-17	297	15
35452.059	.02	63	49	5	3.8	-17	297	15
35731.187	.02	63	49	5	2.1	-17	297	15
35803.387	.02	65	51	4	2.1	-17	297	15
35817.63	.20	64	49	2	3.8	-17	297	15
35859.305	.02	59	45	4	2.1	-16	298	15
35866.484	.02	61	47	5	3.4	-16	297	15
35873.622	.02	59.0	44.7	5	3.8	-16	298	15
35880.963	.02	62	48	5	3.8	-16	298	15
35886.574	.05	63	49	4	3.8	-16	298	15
35910.625	.02	56	52	4	2.1	-16	298	15

NAME: TETRAHYDROTHIOPHENE			CONTINUED			ID NO. 805.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
35994.060	.02	64	50	4	3.0	-16	298	15
36037.983	.02	62	48	5	3.4	-16	298	15
36173.701	.02	64	50	5	2.1	-16	298	15
36395.255	.02	62	47	4	3.0	-16	298	15
36426.653	.02	64	50	5	2.6	-16	297	15
36833.466	.02	64	49	5	1.7	-16	297	15
36848.715	.02	62	47	5	2.1	-15	297	15
36892.292	.02	63	48	5	2.6	-16	297	14
37367.538	.02	65	51	4	2.6	-16	297	15
37425.024	.05	65	49	4	2.1	-16	297	15
37826.096	.02	65	51	4	2.1	-16	297	15
37847.217	.02	64	49	4	1.7	-17	297	15
37946.585	.02	63	49	4	3.0	-17	298	15
38339.713	.02	62	47	5	3.0	-16	298	15
38441.422	.05	64	50	4	2.1	-16	298	15
38604.997	.02	64	50	4	3.0	-16	298	15
38696.469	.02	61	47	5	2.6	-16	298	15
38708.545	.02	63	50	5	3.4	-16	298	15
38855.074	.02	64	50	4	3.0	-15	298	15
38992.603	.02	64	50	4	3.0	-15	296	15
39004.77	.20	61	46	3	3.4	-15	296	15
39070.699	.02	62	48	5	3.0	-15	297	15
39173.784	.02	64	49	5	3.0	-15	297	15
39364.68	.20	65	50	3	2.1	-15	297	15
39417.436	.02	62	47	4	2.6	-15	297	15
39443.974	.02	64	49	4	3.0	-15	297	15
39461.825	.02	62	48	5	3.4	-15	297	15
39480.844	.02	59	45	4	3.4	-15	297	15
39574.600	.02	64	50	5	3.8	-14	298	15
39580.525	.02	66	51	5	2.1	-14	298	15
39608.020	.02	63	48	5	3.8	-15	298	15
39637.860	.02	61	46	5	3.0	-15	298	15
39661.028	.02	62	48	5	3.8	-15	298	15
39737.252	.02	62	47	5	3.0	-14	298	15

## Thiazole

Formula: SCH:NCH:CH

CAS Registry number: 288-47-1

NBS identification number: 169.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich 15,164-5. Sample identity was verified by the manufacturer with gas chromatography and infrared analysis. Chromatography on a Chromosorb 102 column showed only a single impurity of 0.1 percent, which may have been water.

Remarks.- The 10-millitorr operating pressure was registered as 25 millitorr on a thermocouple gage.

NAME: THIAZOLE

ID NO. 169.00

$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
27819.286	.01	60.0	46.3		2.1	-18	296	10
28199.303	.01	57.4	43.5		3.0	-19	297	10
29564.155	.02	58	44	4	2.1	-18	297	10
30349.918	.02	59	45	4	3.8	-17	297	10
30417.968	.01	59.6	45.8		3.0	-17	297	10
30570.571	.02	57	43	4	2.1	-17	297	10
31354.676	.01	59.3	45.6		2.1	-16	297	11
31567.343	.02	61	47	4	3.8	-16	297	11
31984.909	.01	59.4	45.7		3.0	-16	297	10
32137.127	.02	60	46	4	3.0	-16	297	10
32261.168	.01	59.6	45.8		2.1	-16	298	10
32491.131	.01	56.0	42.3		2.1	-16	298	10
33314.592	.02	58	44	4	2.1	-15	298	10
33720.047	.01	60.1	46.8		2.1	-16	298	10
33841.812	.01	55.6	41.9		2.1	-15	298	10
34181.639	.05	57	43	4	3.4	-16	298	10
34744.99	.10	59	45	2	3.0	-16	298	10
34937.298	.01	56	42	4	2.1	-18	298	10
36150.10	.10	60	46	3	3.0	-16	298	10
36178.43	.10	60	46	3	3.0	-16	298	10
36723.819	.01	55	42	4	3.8	-17	298	10
36885.211	.02	56	41	4	3.0	-17	298	10
36888.749	.01	55.6	42.2		3.8	-16	296	10
37025.977	.01	54.6	40.7		2.1	-17	297	10
37252.355	.01	54.3	40.4		2.1	-18	297	10
38341.53	.10	58	45	3	2.1	-17	297	10
39481.078	.02	55	40	4	3.0	-17	297	10
39514.985	.02	56	42	4	2.1	-17	297	10
39751.42	.10	58	44	2	3.4	-17	297	10



## Thietane

Formula:  $\text{CH}_2\text{CH}_2\text{CH}_2\text{S}$

CAS Registry number: 287-27-4

Synonym: trimethylene sulfide

NBS identification number: 193.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman 7877. Chromatography on a Chromosorb 102 column showed impurities of 0.01, 0.06, and 0.08 percent.

Remarks.- The sample identity was confirmed by matching six of the observed lines to theoretically assigned transitions (ref. 7).

The sample pressure of 12 millitorr was registered by a thermocouple gage as 33 millitorr.

NAME: THIETANE					ID NO. 193.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26510.915	.05	65	52	4	2.6	-18	297	12
26705.240	.02	63	50	5	2.1	-18	298	12
26769.106	.05	69	54	4	1.7	-19	298	12
26783.793	.02	65	51	5	3.4	-18	298	12
26844.638	.02	61	47	4	3.4	-18	298	12
27267.044	.02	66	52	4	3.4	-18	296	12
27317.772	.02	62	48	4	2.1	-18	296	12
27319.967	.02	68	54	5	3.4	-18	296	12
27330.301	.02	64	50	4	2.6	-18	297	12
27507.064	.02	67	54	4	1.7	-19	297	12
27524.130	.02	64	50	4	1.7	-19	297	12
27546.591	.02	66	52	4	1.7	-19	297	12
27583.203	.02	62	47	4	2.6	-18	297	12
27901.590	.05	67	54	4	2.6	-18	297	12
27915.874	.02	63	49	5	2.6	-18	297	12
27935.295	.02	62	48	4	2.1	-18	297	12
27956.503	.02	66	52	5	2.1	-18	297	12
28165.343	.02	63	49	4	1.7	-19	297	12
28167.132	.01	64	50	5	2.6	-19	297	12
28354.694	.02	65	52	4	3.0	-17	297	12
28358.52	.10	60	45	3	2.6	-17	297	12
28513.203	.02	68	54	4	2.1	-18	297	12
28538.499	.02	61	48	5	2.1	-17	298	12
28561.980	.01	63	49	5	2.1	-18	298	12
28587.734	.02	65	51	4	2.1	-18	298	12
28847.537	.02	68	53	5	2.1	-18	298	12
28869.952	.02	62	48	4	2.1	-18	298	12
28903.444	.05	67	53	4	2.6	-18	298	12
28905.567	.01	62	49	5	2.6	-18	298	12
28939.690	.02	66	53	5	2.1	-18	298	12
28998.631	.02	68	55	5	1.7	-17	298	12
29026.284	.02	67	53	4	2.1	-17	298	12
29092.356	.02	66	52	5	1.7	-17	298	12
29135.173	.02	65	51	5	3.4	-17	298	12
29160.135	.02	67	53	4	2.6	-17	298	12
29280.774	.05	65	51	5	2.15	-17	298	12
29314.926	.02	68	55	4	2.6	-17	298	12
29350.646	.02	66	51	4	3.4	-17	298	12
29386.050	.02	64	49	5	2.1	-17	298	12
29479.670	.02	65	50	5	1.7	-19	296	12
29483.23	.10	68	53	3	1.7	-19	297	12
29509.441	.05	69	54	4	2.1	-19	297	12
29559.11	.10	62	47	2	2.6	-19	297	12
29562.939	.05	66	51	4	3.0	-19	297	12
29564.942	.01	61	46	5	2.6	-19	297	12
29890.113	.02	64	51	5	2.1	-19	297	12
29943.72	.10	65	51	3	3.0	-19	297	12
29944.665	.02	63	49	4	2.6	-19	297	12
29946.398	.02	66	51	5	3.0	-19	297	12
29956.588	.02	64	50	5	2.6	-19	297	12

NAME: THIETANE		CONTINUED				ID NO. 193.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
30107.605	.02	65	51	5	2.1	-19	297	12
30202.210	.02	65	51	4	3.0	-19	298	12
30233.89	.10	67	54	4	2.15	-19	298	12
30389.071	.01	62	48	5	2.1	-18	298	12
30398.191	.02	67	53	5	3.8	-18	298	12
30455.845	.02	66	52	5	3.4	-18	298	12
30492.809	.02	64	50	4	3.4	-18	298	12
30589.583	.02	63	49	5	2.6	-18	298	12
30592.926	.02	67	52	5	2.6	-18	298	12
30679.408	.01	61	47	5	3.0	-18	298	12
30779.292	.02	60.3	45.9		3.0	-17	297	12
30824.430	.02	68	56	4	1.7	-17	297	12
30839.211	.05	69	54	4	2.6	-17	297	12
30875.187	.02	63	50	5	2.6	-17	297	12
30951.799	.02	65	52	4	2.1	-17	297	12
31165.307	.02	61	46	5	2.1	-18	298	12
31625.465	.05	68	54	4	1.7	-18	297	12
31799.577	.02	67	53	4	2.6	-17	297	12
31858.097	.02	68	54	5	2.6	-17	298	12
31925.790	.02	65	52	4	2.6	-17	298	12
32056.969	.02	69	55	5	1.7	-17	298	12
32275.011	.02	68	55	5	1.7	-17	298	12
32309.625	.02	67	53	4	3.0	-17	298	12
33063.076	.02	60	46	4	2.1	-18	298	12
33190.110	.05	68	53	4	2.6	-17	298	12
33218.604	.02	66	51	4	3.0	-17	298	12
33235.144	.05	67	54	4	1.7	-17	298	12
33274.060	.02	65	50	4	2.6	-19	298	12
33297.085	.02	63	49	5	2.1	-19	298	12
33320.915	.02	62	47	4	2.1	-19	298	12
33344.422	.02	63	48	5	1.7	-19	298	12
33388.889	.02	66	52	4	2.6	-19	298	12
33393.763	.02	63	50	5	2.6	-19	298	12
33414.07	.10	64	50	3	3.0	-19	298	12
33414.66	.10	68	53	2	3.0	-19	298	12
33521.304	.02	68	54	5	2.6	-18	298	12
33533.585	.02	63	49	5	2.1	-18	298	12
33539.521	.02	64	51	4	3.4	-18	298	12
33656.529	.02	67	53	5	3.8	-18	298	12
33822.699	.02	61	47	4	2.6	-17	298	12
33859.112	.02	69	55	4	2.6	-18	298	12
33977.456	.02	67	54	4	3.0	-18	298	12
34022.031	.02	69	56	4	2.1	-17	297	12
34075.205	.02	66	52	5	2.1	-18	297	12
34186.828	.02	64	50	5	2.1	-18	297	12
34246.453	.02	66	52	5	2.6	-18	297	12
34504.779	.01	61	47	5	2.6	-18	297	12
34930.468	.02	65	51	4	2.1	-18	297	12
35095.878	.02	67	54	4	3.0	-18	297	12
35113.195	.02	65	51	5	1.7	-18	297	12



NAME: THIETANE		CONTINUED				ID NO. 193.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
35265.463	.02	64	50	5	2.1	-18	297	12
35267.119	.05	66	52	4	3.8	-18	297	12
35509.337	.01	61	47	5	2.1	-18	298	12
35605.803	.02	67	54	4	2.1	-18	298	12
35924.407	.05	67	52	4	2.1	-18	298	12
35945.563	.02	65	50	5	2.1	-16	298	12
35950.098	.02	64	50	5	2.6	-16	298	12
35957.346	.02	64	49	5	1.7	-16	298	12
35970.015	.02	58	43	4	2.6	-16	298	12
35776.825	.02	62	47	4	1.7	-16	298	12
35992.45	.10	66	51	3	2.1	-16	298	12
35993.27	.10	66	51	2	2.1	-16	298	12
35997.210	.02	67	53	5	2.1	-16	298	12
36012.071	.02	64	49	5	2.1	-17	295	12
36017.401	.01	60.2	45.7		2.1	-17	298	12
36036.479	.02	64	49	5	2.1	-17	298	12
36039.798	.05	63	48	4	3.4	-17	298	12
36127.897	.02	57	54	5	2.1	-16	298	12
36168.003	.02	63	50	5	2.1	-16	298	12
36236.013	.01	59.7	45.3		2.6	-16	298	12
36377.369	.02	66	54	5	2.1	-16	298	12
36425.971	.02	64	50	4	3.0	-16	297	12
36568.619	.01	62	49	5	2.1	-17	297	12
36617.586	.05	67	53	4	2.1	-17	297	12
36675.886	.02	66	51	4	2.1	-17	297	12
36769.013	.01	61	47	5	2.1	-17	297	12
36778.621	.02	67	54	5	1.7	-17	297	12
36953.024	.02	63	48	5	2.1	-17	297	12
36933.880	.02	65	52	4	2.6	-17	297	12
37138.726	.01	61	47	5	2.1	-17	298	12
37343.085	.02	65	51	5	2.1	-17	298	12
37363.739	.02	65	52	5	2.1	-17	298	12
37397.624	.02	64	50	5	2.6	-17	298	12
37452.865	.02	66	52	5	2.1	-17	298	12
37626.145	.02	57	53	5	1.7	-17	298	12
37631.883	.01	59.4	45.1		3.0	-18	298	12
37992.537	.02	68	54	5	2.1	-16	298	12
38075.218	.02	68	55	5	2.1	-16	298	12
38131.895	.02	62	48	5	3.0	-16	298	12
38244.236	.02	64	50	4	2.6	-17	298	12
38281.078	.02	59	56	4	2.6	-17	298	12
38296.160	.02	65	51	4	1.7	-17	298	12
38307.058	.01	62	49	5	2.1	-17	298	12
38311.225	.02	60.3	45.8		3.0	-17	298	12
38326.665	.01	62	48	5	1.7	-17	298	12
38346.265	.02	67	53	4	2.1	-17	298	12
38374.614	.02	66	52	5	3.4	-17	298	12
38435.080	.02	69	55	5	2.1	-17	298	12
38525.108	.01	62	48	5	3.4	-17	298	12
38529.952	.02	65	52	5	2.6	-16	298	12

NAME: THIEANE			CONTINUED			ID NO. 193.00		
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
38551.059	.02	67	54	4	2.1	-16	298	12
38573.570	.01	59.9	45.6		3.8	-17	298	12
38600.578	.02	63	49	5	2.1	-17	298	12
38646.563	.02	65	51	5	3.0	-16	298	12
38707.766	.02	61	47	4	3.4	-16	298	12
38715.149	.02	64	50	4	3.4	-17	298	12
38721.558	.02	69	55	4	2.1	-17	298	12
38753.933	.02	64	50	4	3.0	-16	297	12
38822.616	.02	58	45	4	2.1	-16	298	12
38825.625	.01	56.6	42.4		3.8	-16	298	12
38846.095	.02	67	53	4	1.7	-17	298	12
38887.558	.01	60.2	46.7		3.4	-17	298	12
39069.400	.02	63	49	5	3.4	-16	298	12
39119.681	.02	61	46	5	3.4	-16	298	12
39150.793	.01	61	47	5	2.6	-16	298	12
39210.621	.02	67	53	5	2.1	-16	298	12
39260.765	.01	59.8	45.6		3.0	-16	298	12
39269.353	.02	63	49	5	2.6	-16	298	12
39296.373	.05	69	56	4	2.1	-16	298	12
39310.473	.02	65	51	5	2.6	-16	298	12
39334.869	.02	67	53	4	2.6	-16	298	12
39338.184	.02	60.2	46.2		3.0	-16	298	12
39363.731	.02	63	50	4	2.6	-16	298	12
39376.326	.05	67	53	4	2.6	-16	298	12
39384.247	.01	57.6	43.5		3.0	-16	298	12
39391.709	.01	56.5	42.4		2.6	-16	298	12
39418.112	.02	66	52	5	2.1	-16	298	12
39430.173	.02	62	49	5	2.1	-16	298	12
39464.421	.02	64	50	5	1.7	-16	298	12
39478.782	.02	65	51	4	2.1	-16	298	12
39655.381	.02	67	53	4	2.1	-17	298	12
39958.487	.01	58.6	44.4		3.0	-19	298	12

## Thiirane

Formula:  $\text{SCH}_2\text{CH}_2$

CAS Registry number: 420-12-2

Synonym: ethylene sulfide

NBS identification number: 324.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Aldrich 12,825-2 with a stated purity of 99+ percent. Sample identity was verified by the manufacturer from gas chromatography and infrared analysis. Chromatography on a Chromosorb 102 column showed impurities of 0.36, 0.15, and 1.02 percent.

Remarks.- The identity of the sample was confirmed by matching four of the lines with theoretical transitions. In addition, the approximate frequency of several more of the lines has been previously reported (ref. 3).

The 15-millitorr sample pressure was registered as 34 millitorr by a thermo-couple gage.

NAME: THIIRANE					ID NO. 324.00			
$\nu_0$ , MHz	U, MHz	$-10 \log \gamma$	$-10 \log \frac{\gamma \Delta \nu}{p}$	Line- type code	$E_s$ , kV/cm	P, dBm	T, K	p, mtorr
26973.154	.02	55	42	4	3.0	-18	300	15
27118.859	.01	55.9	42.2		3.0	-18	299	15
27648.283	.01	58.9	45.7		3.0	-18	299	15
28033.587	.01	58.9	46.7		2.1	-18	300	15
28723.131	.01	53.0	39.2		3.0	-19	300	15
29336.576	.01	51.8	38.4	4	3.0	-18	299	15
29924.072	.01	54.4	40.4		3.0	-20	298	15
30439.399	.01	53.7	40.0		3.4	-19	298	15
30559.768	.01	51.5	37.6		2.0	-18	298	15
34243.233	.01	54.9	42.2		3.0	-17	298	15
34903.429	.02	53	38	4	2.1	-17	298	15
35515.265	.02	52	39	4	3.0	-17	298	15
37238.217	.02	48.7	34.5	4	2.1	-17	298	15
37281.856	.01	55.6	42.6		3.8	-17	298	15
37238.216	.02	48.9	34.5		2.1	-16	298	15

## Thiophene

Formula: SCH:CHCH:CH

CAS Registry number: 110-02-1

Synonym: thiofuran

NBS identification number: 212.00

Frequency range: 26 500 to 40 000 MHz

Sample.- The sample was Eastman 1860. Chromatography on a Chromosorb 102 column showed two impurities of less than 0.1 percent each.

Remarks.- These lines are narrow and most of them require high modulating fields. Some could not be completely modulated at the highest available field (3.8 kV/cm).

Sample identity was verified by matching only one line with theoretical transitions (ref. 3). A second transition has been reported, but the intensity was below the threshold used for the scan. Data were also compared with an earlier spectral recording made on the Tracerlab spectrometer.

The sample pressure of 15 millitorr was registered as 42 millitorr by a thermocouple gage.

NAME: THIOPHENE					ID NO. 212.00			
$\nu_0$ , MHz	U, MHz	-10 log $\gamma$	-10 log $\frac{\gamma \Delta \nu}{p}$	Line- type code	E <sub>s</sub> , kV/cm	P, dBm	T, K	p, mtorr
26810.297	.05	68	59	5	2.6	-20	297	15
26957.815	.02	66	56	5	3.8	-19	297	15
27632.489	.02	65	56	5	2.6	-18	297	15
28065.267	.05	68	59	4	2.6	-18	297	15
28211.516	.02	63	53	5	3.4	-19	297	15
28399.972	.02	67	57	5	3.4	-18	297	15
28488.883	.02	65	55	5	3.8	-18	297	15
28879.896	.02	65	55	5	3.0	-18	297	15
28967.725	.05	65	56	4	3.8	-18	297	15
29102.537	.02	64	55	5	3.4	-18	297	15
29228.105	.02	65	55	5	3.4	-18	297	15
29317.385	.02	61	52	4	3.8	-18	297	15
29729.492	.02	65	56	4	3.0	-19	298	15
30025.416	.01	62	53	5	3.4	-20	298	15
30269.755	.01	63	54	4	3.0	-19	298	15
30619.623	.01	64	55	5	3.4	-18	298	15
30711.853	.01	65	55	5	3.8	-18	298	15
31025.702	.01	62	52	5	3.8	-17	298	15
31043.982	.02	62	53	4	3.4	-17	298	15
31254.032	.01	64	55	5	3.4	-18	298	15
31257.825	.01	64	55	5	3.0	-18	298	15
31329.561	.01	62	53	5	3.4	-18	298	15
31345.746	.01	64	55	5	3.8	-18	298	15
30025.418	.01	62	53	5	3.8	-19	298	15
32374.122	.02	67	57	4	2.1	-18	297	15
32418.364	.02	66	56	4	3.8	-19	297	15
33880.136	.01	61	51	5	3.8	-18	297	15
34265.335	.02	65	56	4	3.8	-17	297	15
34641.232	.02	68	59	4	3.8	-17	297	15
35388.157	.01	65	55	5	3.0	-18	297	15
35552.123	.02	61	53	4	3.8	-17	297	15
35664.869	.01	59	50	4	3.8	-17	298	15
35899.328	.01	65	55	5	3.0	-17	298	15
36346.305	.01	62	53	5	3.8	-17	298	15
36817.193	.02	66	57	4	3.8	-16	298	15
36856.308	.01	62	53	5	3.8	-16	298	15
37250.522	.01	65	55	5	2.1	-17	298	15
39056.135	.01	67	57	5	2.6	-17	298	15
39117.167	.01	60	50	4	3.8	-17	298	15
39142.680	.01	63	54	4	3.8	-17	298	15
39377.577	.02	67	58	4	2.6	-17	298	15
39736.894	.02	69	59	4	1.7	-17	298	15

## CONCLUDING REMARKS

The spectra presented in this report are not represented as being complete, since in most cases the spectrometer was programed to ignore lines with an absorption coefficient less than the low to mid  $10^{-7}$   $\text{cm}^{-1}$  range. It would be desirable to include all detectable lines in a catalog intended for analytical use, but the time required precluded this. The intensity cutoff limit chosen is a compromise to allow measurements to be made on a larger number of molecules. At the same time, the information included in the tables is more than adequate to allow qualitative, and in most cases quantitative, analysis of samples containing any of the tabulated molecules, even in a complex mixture. In general, though, it will not be possible to identify all the observed spectral lines in a scan of a given frequency range, even for a pure compound. One recommended use of the data is to search only for the stronger lines of a compound and to use a process of elimination to determine which of the tabulated compounds are present in the sample. In that way the absence of one of the compounds can be determined by observing a lack of signal at a single frequency.

The data in this report include only a portion of the spectra which have been measured to date. The choice of sulfur and nitrogen compounds as a class for this report was made because some of these are of importance in air-pollution studies. Other categories for which spectra were measured include volatile organic compounds and chlorinated or fluorinated compounds.

In order to make microwave spectroscopy a truly useful analytical tool, it will be necessary to increase vastly the amount of available reference data. It is hoped that the publication of this first catalog will serve to stimulate more interest and activity in this promising area and that other laboratories will begin to contribute to the store of analytical reference spectra.

Langley Research Center,  
National Aeronautics and Space Administration,  
Hampton, Va., February 4, 1974.

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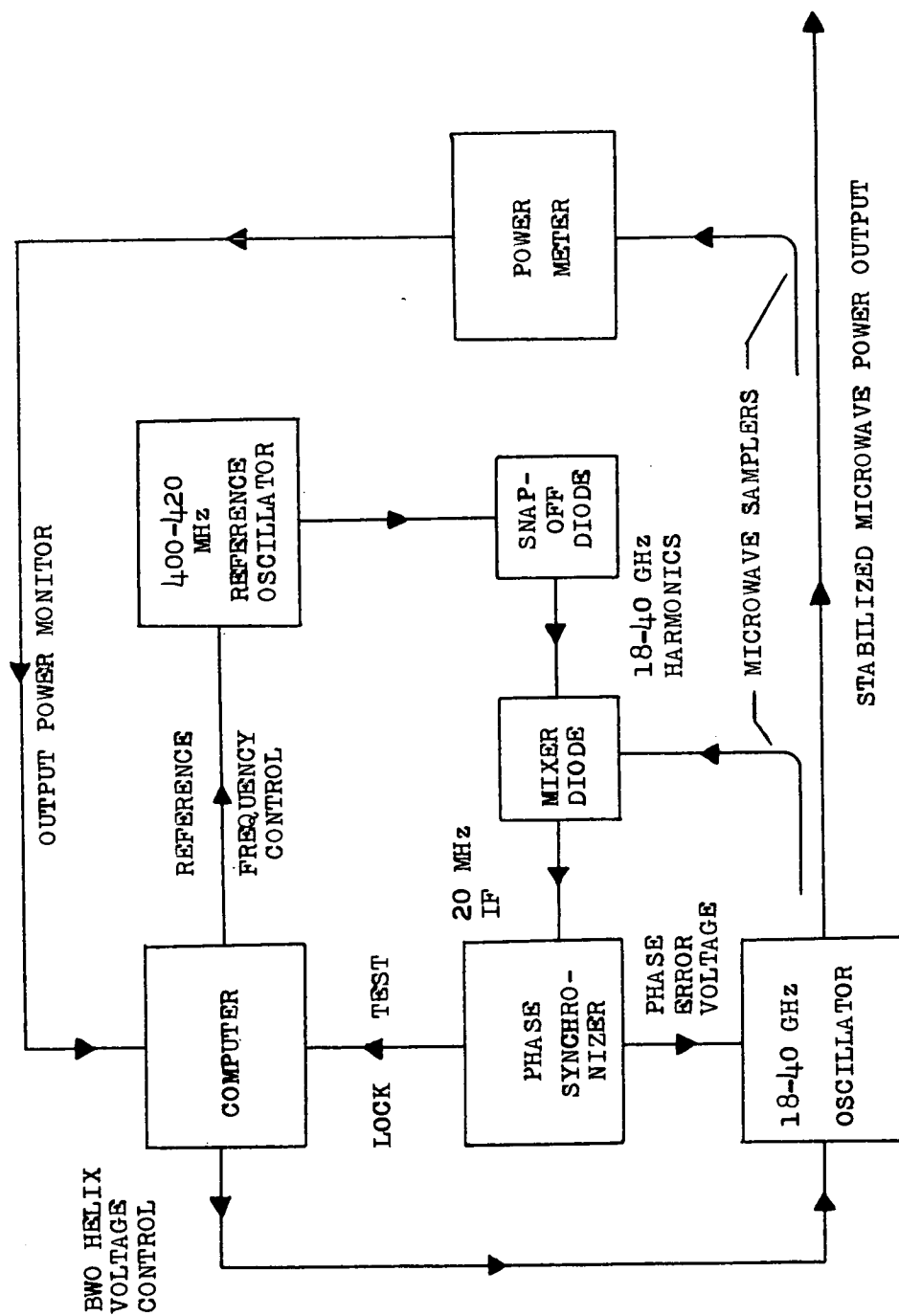


Figure 1.- Stabilized digital microwave source.

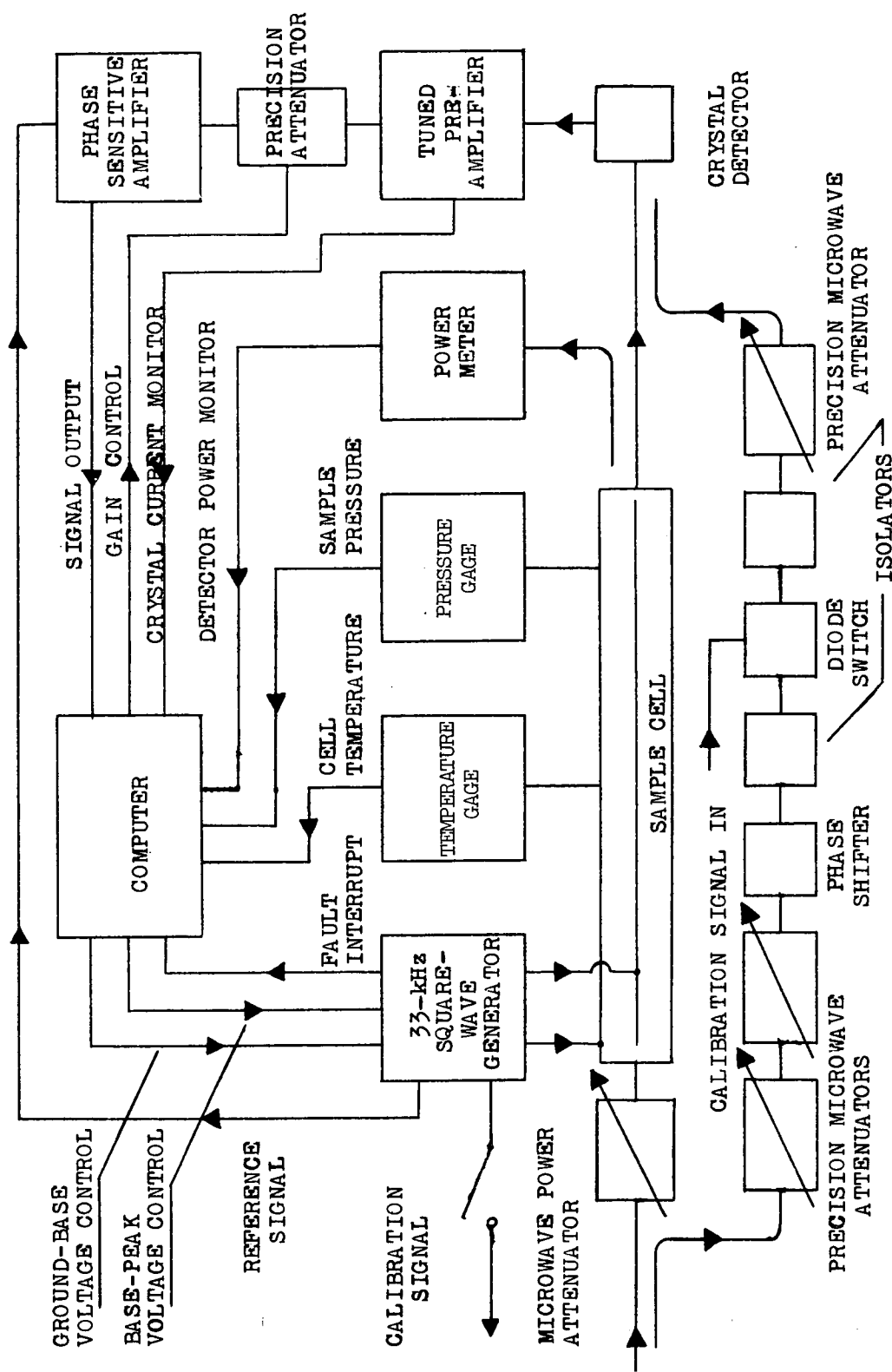
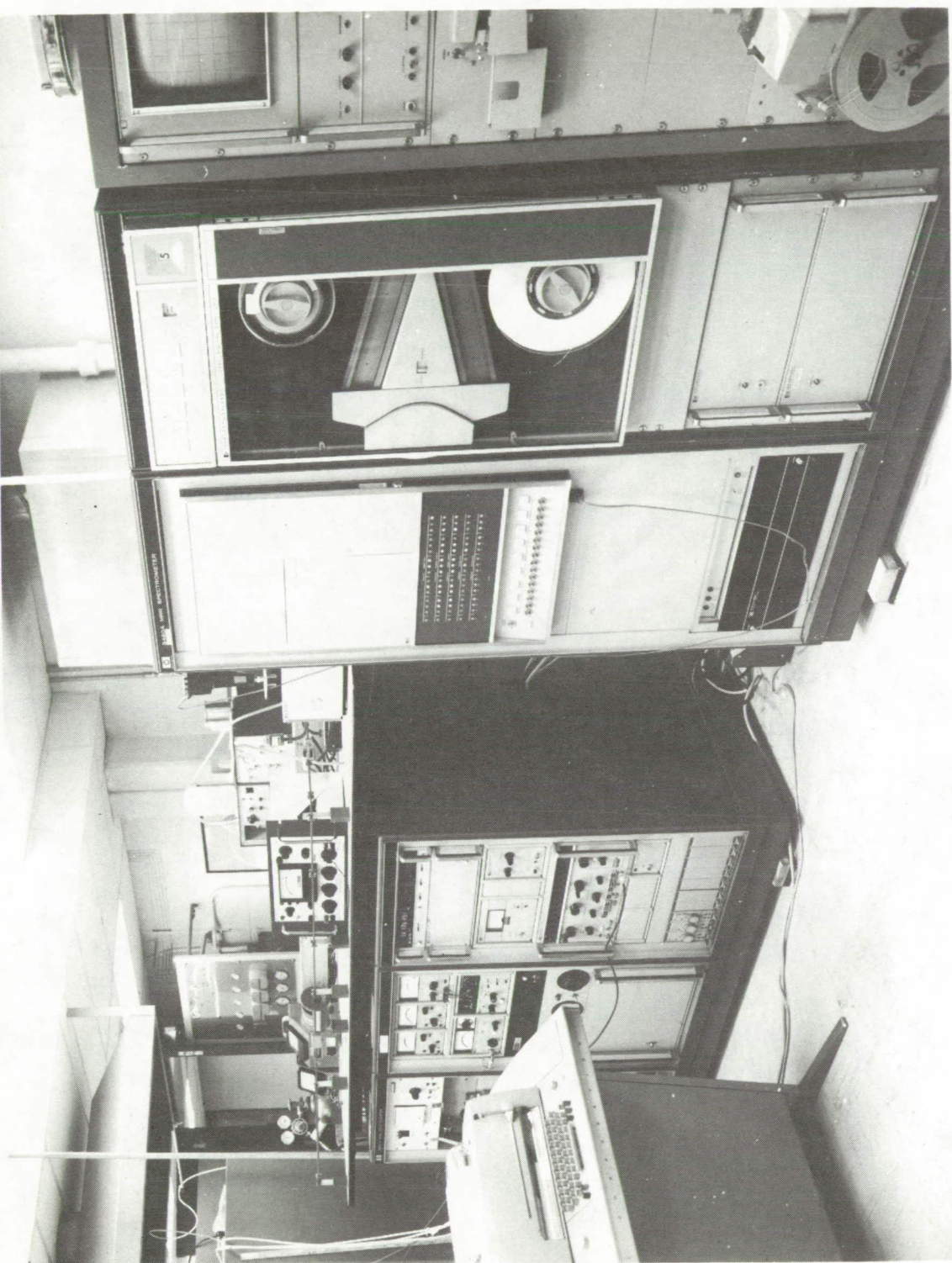


Figure 2.- Detection, modulation, calibration, and status-monitoring system.



L-71-6358

Figure 3.- Computer-controlled microwave spectrometer.



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